Sharp-interface nematic-isotropic phase transitions with flow

Eliot Fried

Department of Mechanical and Aerospace Engineering
Washington University in St. Louis
St. Louis, MO 63130-4899, USA

Abstract

We present a sharp-interface theory for phase transformations between the isotropic and uniaxial nematic phases of a flowing liquid crystal. These equations include a supplemental interface condition which expresses the balance of configurational momentum. As an application, we study the behavior a spherical isotropic drop surrounded by a radially-oriented nematic phase. For this problem, the bulk and interfacial equations collapse to a single nonlinear second-order ordinary differential equation for the radius of the droplet. We determine and study the stability of the corresponding equilibria. In addition, we find that motion of the interface generates a backflow in the nematic phase. Our analysis indicates that a backflow measurement can be used to determine independently the density difference between the isotropic and uniaxial nematic phases.

1 Introduction

In a recent paper, Cermelli, Fried & Gurtin [5] generalized the classical curvature elasticity theory of Oseen [19], Zöcher [25], and Frank [13] to

- allow for phase transitions,
- model a nematic-isotropic interface as a sharp surface across which bulk fields may suffer discontinuities,
- account for localized interactions between phases by endowing the interface with excess properties.

Here, we extend the theory of Cermelli, Fried & Gurtin [5] to account for flow and thereby take another step toward providing a generalization of the Ericksen–Leslie theory (Ericksen [10, 11, 12]; Leslie [16, 17]) appropriate to describing transformations phase transformations between the isotropic and uniaxial nematic phases of a flowing liquid crystal.

Aside from developing governing equations for the bulk phases and the interface, we revisit a simple application studied by Cermelli, Fried & Gurtin [5]. That application involves the growth and equilibrium of a spherical isotropic drop in a nematic ocean in which the director is radially oriented. When flow is accounted for, the solution of this problem involves determining the velocity and pressure fields in the phases. As in the case when flow is neglected, we find that the bulk and interfacial equations collapse to a single nonlinear second-order ordinary differential equation—enforcing the balance of configurational momentum—for the radius of the droplet. On writing R for the radius of the droplet, this equation has the form

$$\frac{[\![v]\!]^2}{v^+v^-}\left\{R\ddot{R}+\frac{3\dot{R}^2}{2}+\frac{4v^-(\mu_1+\mu_4)\dot{R}}{R}+\frac{2v^-(\lambda_1+\lambda_5)\dot{R}}{R^2}\right\}+\frac{\lambda_9\dot{R}}{v^+}=v^-\Psi_0-[\![v]\!]p_\infty-v^+\left\{\frac{2\gamma_0}{R}-\frac{\kappa}{R^2}\right\}, \quad (1.1)$$

where v^+ and v^- denote the specific volumes of the isotropic and nematic phases, $[\![v]\!]=v^+-v^-$, $\mu_1+\mu_4>0$ (with μ_1 and μ_4 determined by the Leslie coefficients α_1, α_4, α_5, and α_6 via $\mu_1=(\alpha_1+\alpha_5+\alpha_6)/3$ and $\mu_4=\alpha_4/2$), $\lambda_1+\lambda_2>0$ is the dilational viscosity of the interface, λ_9 is the reciprocal mobility of the interface, Ψ_0 is the free-energy density of the nematic phase, in a state of uniform alignment, measured relative to the isotropic phase, p_∞ is the pressure in the far-field, γ_0 is the isotropic contribution to the

interfacial free-energy density, and $\kappa = 2k_1 - (k_2 + k_4) \geq 0$, (with k_1, k_2, and k_4 being the classical Frank moduli for splay, twist, bend, and saddle-splay). When the densities of the phases are equal, so that $[\![v]\!] = 0$, (1.1) reduces to an equation with structure identical to that of the equation derived and studied by Cermelli, Fried & Gurtin [5] for the droplet evolution problem without flow. We determine and study the stability of the equilibria of (1.1). Generally, the number and nature of the equilibria is essentially unchanged from the case without flow. With flow taken into account, however, the detailed expressions for the equilibrium states are influenced by the ambient pressure. Additionally, the dynamics of the droplet are evidently influenced by inertia, the viscosity of the nematic phase, and the dilatational viscosity of the interface.

Within the isotropic phase, the velocity is trivial and the pressure is spatially uniform and determined in terms of the radius of the droplet and relevant material parameters. Within the nematic phase, the velocity and pressure are determined in terms of the radius of the droplet, with the velocity being radial. Whereas the velocity decays is inversely proportional to the square of the distance from the origin, in the far-field the pressure tends toward a uniform ambient value.

Most importantly, when flow is taken into account, we find that motion of the interface generates a backflow in the nematic phase. Writing $\mathbf{u}^-$ for the interfacial limit of the velocity of the nematic phase, $\mathfrak{m}$ for the interfacial unit normal (directed into the isotropic phase), we find in particular that

$$\frac{[\![v]\!]}{v^+} = -\frac{\mathbf{u}^- \cdot \mathfrak{m}}{\dot{R}}.$$

Our analysis therefore shows that a backflow measurement provides an independent means to measure the density difference between the phases.

2 Theory for the nematic phase

The theory for the nematic phase is a specialization of the Ericksen–Leslie theory (Ericksen [10, 11, 12]; Leslie [16, 17]) to a setting in which thermal transport is neglected.

The basic kinematical descriptors of the theory are the *velocity* $\mathbf{u}$ and the *director* $\mathbf{n}$. We write

$$\mathbf{L} = \operatorname{grad} \mathbf{u} \qquad \text{and} \qquad \mathbf{G} = \operatorname{grad} \mathbf{n}$$

for the *velocity gradient* and the *director gradient* and

$$\mathbf{D} = \tfrac{1}{2}(\mathbf{L} + \mathbf{L}^\top) \qquad \text{and} \qquad \mathbf{W} = \tfrac{1}{2}(\mathbf{L} - \mathbf{L}^\top)$$

for the *rate of stretch* and the *rate of spin*. As is standard, we assume that the nematic phase is incompressible, so that

$$\operatorname{div} \mathbf{u} = \operatorname{tr} \mathbf{L} = 0. \tag{2.1}$$

Further, since the director describes the axis of the uniaxial nematic order tensor, we assume that

$$|\mathbf{n}| = 1 \tag{2.2}$$

and that $\mathbf{n}$ and $-\mathbf{n}$ are indistinguishible.

We use a superposed dot to denote *material time-differentiation*; e.g., for a scalar field Φ, $\dot{\Phi} = \partial\Phi/\partial t + (\operatorname{grad}\Phi)\cdot\mathbf{u}$. Aside from the constraints (2.1) and (2.2), the governing equations in the nematic phase are then

$$\left.\begin{aligned} \varrho\dot{\mathbf{u}} &= -\operatorname{grad} p - \operatorname{div}\left\{\mathbf{G}^\top \frac{\partial \Psi}{\partial \mathbf{G}}\right\} + \operatorname{div}\mathbf{T}_{\rm dis}, \\ \sigma(\ddot{\mathbf{n}} + |\dot{\mathbf{n}}|^2\mathbf{n}) &= \operatorname{div}\left\{\frac{\partial \Psi}{\partial \mathbf{G}}\right\} + \left\{\mathbf{G} \colon \frac{\partial \Psi}{\partial \mathbf{G}}\right\}\mathbf{n} - \frac{\partial \Psi}{\partial \mathbf{n}} + \mathbf{g}_{\rm dis}, \end{aligned}\right\} \tag{2.3}$$

where ϱ is the (constant) mass density, σ is the (constant) director mass density (i.e., the peculiar mass density of a mesogen), p is the pressure required to maintain the constraint (2.1), Ψ is the *free-energy*

(*density*), as given FRANK's [13] quadratic expression[1]

$$\Psi = \Psi_0 + \tfrac{1}{2}k_1(\mathsf{div}\,\mathbf{n})^2 + \tfrac{1}{2}k_2(\mathbf{n}\cdot\mathsf{curl}\,\mathbf{n})^2 + \tfrac{1}{2}k_3|\mathbf{n}\times\mathsf{curl}\,\mathbf{n}|^2 + \tfrac{1}{2}(k_2+k_4)(\mathsf{tr}\,((\mathsf{grad}\,\mathbf{n})^2) - (\mathsf{div}\,\mathbf{n})^2), \quad (2.4)$$

and $\mathbf{T}_{\rm dis}$ and $\mathbf{g}_{\rm dis}$ are given by (ERICKSEN [11]; LESLIE [16])[2]

$$\left.\begin{aligned}\mathbf{T}_{\rm dis} &= \mu_1(\mathbf{n}\cdot\mathbf{D}\mathbf{n})(3\mathbf{n}\otimes\mathbf{n}-\mathbf{1}) + \mu_2\boldsymbol{\omega}\otimes\mathbf{n} + \mu_3\mathbf{n}\otimes\boldsymbol{\omega} + 2\mu_4\mathbf{D}\\ &\quad + 2\mu_5(\mathbf{1}-\mathbf{n}\otimes\mathbf{n})\mathbf{D}\mathbf{n}\otimes\mathbf{n} + 2\mu_6\mathbf{n}\otimes(\mathbf{1}-\mathbf{n}\otimes\mathbf{n})\mathbf{D}\mathbf{n},\\ \mathbf{g}_{\rm dis} &= -(\mu_3-\mu_2)\boldsymbol{\omega} - 2(\mu_6-\mu_5)(\mathbf{1}-\mathbf{n}\otimes\mathbf{n})\mathbf{D}\mathbf{n},\end{aligned}\right\} \quad (2.5)$$

where $\boldsymbol{\omega} = \dot{\mathbf{n}} - \mathbf{W}\mathbf{n}$ and the viscosities μ_1, μ_2, μ_3, μ_4, and μ_5 obey

$$\left.\begin{aligned}&\mu_1+\mu_4>0, \qquad \mu_3>\mu_2, \qquad \mu_4>0, \qquad 2\mu_4+\mu_5+\mu_6>0,\\ &(\mu_3-\mu_2)(2\mu_4+\mu_5+\mu_6) > 2(\mu_2+\mu_3+2\mu_6-2\mu_5)^2.\end{aligned}\right\} \quad (2.6)$$

Granted (2.4) and (2.5), the equations (2.3) may be recast in the compact form[3]

$$\left.\begin{aligned}\dot{\mathbf{p}} &= \mathsf{div}\,\mathbf{T},\\ \dot{\mathbf{r}} &= \mathsf{div}\,\mathbf{S} + \mathbf{g},\end{aligned}\right\} \quad (2.7)$$

where $\mathbf{p} = \varrho\mathbf{u}$ is *linear momentum*, $\mathbf{T}$ is the *Cauchy stress*, $\mathbf{r} = \sigma\dot{\mathbf{n}}$ is *director momentum*, $\mathbf{S}$ is the *director stress*, and $\mathbf{g}$ is the *director body force* (*density*), given by the constitutive relations[4]

$$\left.\begin{aligned}\mathbf{T} &= -p\mathbf{1} - \mathbf{G}^\top\mathbf{S} + \mathbf{T}_{\rm dis},\\ \mathbf{S} &= \mathbf{n}\otimes\boldsymbol{\alpha} + \frac{\partial\Psi}{\partial\mathbf{G}},\\ \mathbf{g} &= \beta\mathbf{n} - \mathbf{G}\boldsymbol{\alpha} - \frac{\partial\Psi}{\partial\mathbf{n}} + \mathbf{g}_{\rm dis},\end{aligned}\right\} \quad (2.8)$$

with $\boldsymbol{\alpha}$ and β being constitutively indeterminate fields that arise in response to the constraint (2.2).

Granted (2.4), (2.5), and (2.8), it can be verified that

$$\mathbf{T} + \mathbf{S}\mathbf{G}^\top + \mathbf{n}\otimes\mathbf{g} = (\mathbf{T} + \mathbf{S}\mathbf{G}^\top + \mathbf{n}\otimes\mathbf{g})^\top, \quad (2.9)$$

which is equivalent to the balance of angular momentum, and that

$$\dot{\Psi} - (\mathbf{T} + \mathbf{G}^\top\mathbf{S})\cdot\mathbf{L} - \mathbf{S}\cdot\dot{\mathbf{G}} + \mathbf{g}\cdot\dot{\mathbf{n}} \le 0 \quad (2.10)$$

which is the dissipation inequality expressing the first and second laws of thermodynamics under isothermal conditions.

[1] The quantity Ψ_0 contains information about the energy of the nematic phase, in a state of uniform alignment, relative to that of the isotropic phase. For fixed compositions and in the absence of external electromagnetic fields, we might expect Ψ_0 to be negative at sufficiently low temperatures, positive at sufficiently high temperatures, and zero at some intermediate temperature.

[2] The expressions (2.5) for the dissipative contributions $\mathbf{T}_{\rm dis}$ and $\mathbf{g}_{\rm dis}$ to $\mathbf{T}$ and $\mathbf{g}$ are defined consistent with the geometric restrictions $\mathsf{tr}\,\mathbf{T}_{\rm dis} = 0$ and $\mathbf{g}_{\rm dis}\cdot\mathbf{n} = 0$ arising from the constraints (2.1) and (2.2) and therefore differ slightly from the standard expressions given by ERICKSEN [11] and LESLIE [16]. Consistency with the standard expressions involving the Leslie coefficients α_1, α_2, α_3, α_4, α_5, and α_6 is obtained by using the relations $\mu_1 = (\alpha_1+\alpha_5+\alpha_6)/3$, $\mu_2 = \alpha_2$, $\mu_3 = \alpha_3$, $\mu_4 = \alpha_4/2$, $\mu_5 = \alpha_5/2$, and $\mu_6 = \alpha_6/2$ and absorbing the terms $\mu_1(\mathbf{n}\cdot\mathbf{D}\mathbf{n})\mathbf{1}$ and $2(\mu_6-\mu_5)(\mathbf{n}\cdot\mathbf{D}\mathbf{n})\mathbf{n}$ into the reactions $-p\mathbf{1}$ and $\beta\mathbf{n}$.

[3] More precisely, granted that $\mathbf{S}$ and $\mathbf{g}$ are as determined by (2.4) and $(2.8)_{2,3}$, $(2.3)_2$ is equivalent to the projection of $(2.7)_2$ onto the plane orthogonal to $\mathbf{n}$.

[4] The derivatives in (2.8) are defined consistent with the constraint $(2.1)_2$ and thus obey $(\partial\Psi/\partial\mathbf{n})\cdot\mathbf{n} = 0$ and $(\partial\Psi/\partial\mathbf{G})^\top\mathbf{n} = \mathbf{0}$. We avoid a detailed discussion of constraints and associated multiplier fields. A modern geometrical treatment of constraints in a material with nematic microstructure is provided by ANDERSON, CARLSON & FRIED [2] and CHEN & FRIED [7].

3 Configurational momentum and stress in the nematic phase

For homogeneous bulk phases, configurational forces do not describe new physics. When a phase interface is present, however, configurational forces are of essential importance. Moreover, a knowledge of the structure of the bulk configurational forces is central to the understanding of their localized effects at the interface. With this in mind, we now summarize the results of Cermelli & Fried [4] concerning the forms of the bulk configurational momentum and stress in nematic liquid-crystals.

We consider a configurational momentum balance involving three fields: a *configurational momentum* (*density*) $\mathbf{q}$, a *configurational stress* $\mathbf{C}$, and a *configurational body force* (*density*) $\mathbf{f}$. The local form of the balance of configurational momentum is

$$\dot{\mathbf{q}} = \mathsf{div}\,\mathbf{C} + \mathbf{f}. \tag{3.1}$$

Since no changes of material structure occur in bulk, we require that the local configurational balance (3.1) be identically satisfied away from the interface: the bulk force $\mathbf{f}$ is therefore indeterminate, and *defined* by the relation $\mathbf{f} = \dot{\mathbf{q}} - \mathsf{div}\,\mathbf{C}$.

Insight regarding the structure of $\mathbf{p}$ and $\mathbf{C}$ is best obtained using an integral formulation involving control volumes $\mathcal{R}(t)$ that migrate relative to the liquid (Gurtin [14, 15]). One of the advantages of such an approach is that a migrating control volumes can be chosen to evolve following the interface. This observation leads to the notion of a *superficial pillbox* introduced later in Section 6.1.

Let $\mathbf{v}_{\partial\mathcal{R}}$ be a velocity field describing the motion of $\partial\mathcal{R}(t)$, and let $V_{\partial\mathcal{R}}$ the (scalar) normal velocity of $\partial\mathcal{R}$ in the direction of the outward unit normal $\mathbf{m}_{\partial\mathcal{R}}$. To characterize the motion of $\mathcal{R}(t)$ relative to the liquid we use the relative velocities

$$\mathbf{v}^{\rm rel}_{\partial\mathcal{R}} = \mathbf{v}_{\partial\mathcal{R}} - \mathbf{u} \qquad \text{and} \qquad V^{\rm rel}_{\partial\mathcal{R}} = V_{\partial\mathcal{R}} - \mathbf{u}\cdot\mathbf{m}_{\partial\mathcal{R}}.$$

Given a migrating control volume $\mathcal{R}(t)$, the field $\partial\mathbf{n}/\partial t + \mathbf{G}\mathbf{v}_{\partial\mathcal{R}}$ represents the *rate of change of the director following the observed motion of* $\partial\mathcal{R}$. Notice that we may write

$$\frac{\partial\mathbf{n}}{\partial t} + \mathbf{G}\mathbf{v}_{\partial\mathcal{R}} = \dot{\mathbf{n}} + \mathbf{G}\mathbf{v}^{\rm rel}_{\partial\mathcal{R}}.$$

Moreover, since $\mathsf{div}\,\mathbf{u} = 0$, we conclude that for any scalar field Φ

$$\frac{\rm d}{{\rm d}t}\int\limits_{\mathcal{R}(t)} \Phi\,{\rm d}v = \int\limits_{\mathcal{R}(t)} \dot{\Phi}\,{\rm d}v + \int\limits_{\partial\mathcal{R}(t)} \Phi V^{\rm rel}_{\partial\mathcal{R}}\,{\rm d}a. \tag{3.2}$$

By integrating the local laws (2.7), (2.10), and (3.1) over $\mathcal{R}(t)$ and using (3.2) and the divergence theorem, we obtain equivalent expressions for a migrating control volume. To begin with, the balance laws for linear, director, and configurational momentum become

$$\left.\begin{aligned}
\frac{\rm d}{{\rm d}t}\int\limits_{\mathcal{R}(t)} \mathbf{p}\,{\rm d}v &= \int\limits_{\partial\mathcal{R}(t)} \Big\{\mathbf{T}\mathbf{m}_{\partial\mathcal{R}} + \mathbf{p}V^{\rm rel}_{\partial\mathcal{R}}\Big\}\,{\rm d}a,\\
\frac{\rm d}{{\rm d}t}\int\limits_{\mathcal{R}(t)} \mathbf{r}\,{\rm d}v &= \int\limits_{\partial\mathcal{R}(t)} \Big\{\mathbf{S}\mathbf{m}_{\partial\mathcal{R}} + \mathbf{r}V^{\rm rel}_{\partial\mathcal{R}}\Big\}\,{\rm d}a + \int\limits_{\mathcal{R}(t)} \mathbf{g}\,{\rm d}v,\\
\frac{\rm d}{{\rm d}t}\int\limits_{\mathcal{R}(t)} \mathbf{q}\,{\rm d}v &= \int\limits_{\partial\mathcal{R}(t)} \Big\{\mathbf{C}\mathbf{m}_{\partial\mathcal{R}} + \mathbf{q}V^{\rm rel}_{\partial\mathcal{R}}\Big\}\,{\rm d}a + \int\limits_{\mathcal{R}(t)} \mathbf{f}\,{\rm d}v.
\end{aligned}\right\} \tag{3.3}$$

In the form (3.3), the balances suggest a view of $\mathbf{T}\mathbf{m}_{\partial\mathcal{R}} + \mathbf{p}V^{\rm rel}_{\partial\mathcal{R}}$, $\mathbf{S}\mathbf{m}_{\partial\mathcal{R}} + \mathbf{r}V^{\rm rel}_{\partial\mathcal{R}}$, and $\mathbf{C}\mathbf{m}_{\partial\mathcal{R}} + \mathbf{q}V^{\rm rel}_{\partial\mathcal{R}}$ as *effective tractions* (Cermelli & Fried [3]), a view that we take when we discuss the configurational form of the energy inequality for a migrating control volume.

Using the identity $\dot{\mathbf{G}} = \mathsf{grad}\,(\dot{\mathbf{n}}) - \mathbf{G}\mathbf{L}$ and the local laws (2.7), we next rewrite (2.10) as a local energy inequality:

$$\dot{\Psi} + \varrho\mathbf{u}\cdot\dot{\mathbf{u}} + \sigma\dot{\mathbf{n}}\cdot\ddot{\mathbf{n}} \le \mathsf{div}\Big\{\mathbf{T}^{\top}\mathbf{u} + \mathbf{S}^{\top}\dot{\mathbf{n}}\Big\}. \tag{3.4}$$

Integrating (3.4) over $\mathcal{R}(t)$ and using (3.2) and the divergence theorem, we obtain an energy inequality

$$\frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\mathcal{R}(t)}\left\{\Psi+\tfrac{1}{2}\varrho|\mathbf{u}|^2+\tfrac{1}{2}\sigma|\dot{\mathbf{n}}|^2\right\}\mathrm{d}v\leq\int\limits_{\partial\mathcal{R}(t)}\left\{\mathbf{T}\mathbf{m}_{\partial\mathcal{R}}\cdot\mathbf{u}+\mathbf{S}\mathbf{m}_{\partial\mathcal{R}}\cdot\dot{\mathbf{n}}+(\Psi+\tfrac{1}{2}\varrho|\mathbf{u}|^2+\tfrac{1}{2}\sigma|\dot{\mathbf{n}}|^2)V^{\mathrm{rel}}_{\partial\mathcal{R}}\right\}\mathrm{d}a \tag{3.5}$$

for a migrating control volume. This inequality accounts only *implicitly* for the power expended by configurational forces. We now give an equivalent alternative of the energy inequality that accounts *explicitly* for power expended by configurational forces. In this regard it is important to bear in mind that in contrast to a control volume that convects with the liquid, a control volume $\mathcal{P}(t)$ that migrates with respect to the liquid has no intinsic physical meaning. Consistent with this and the conventional version

$$\frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\mathcal{P}(t)}\left\{\Psi+\tfrac{1}{2}\varrho|\mathbf{u}|^2+\tfrac{1}{2}\sigma|\dot{\mathbf{n}}|^2\right\}\mathrm{d}v\leq\int\limits_{\partial\mathcal{P}(t)}\left\{\mathbf{T}\mathbf{m}_{\partial\mathcal{R}}\cdot\mathbf{u}+\mathbf{S}\mathbf{m}_{\partial\mathcal{R}}\cdot\dot{\mathbf{n}}\right\}\mathrm{d}a \tag{3.6}$$

of the energy inequality, we rewrite the energy inequality for $\mathcal{R}(t)$ in the form

$$\frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\mathcal{R}(t)}\left\{\Psi+\tfrac{1}{2}\varrho|\mathbf{u}|^2+\tfrac{1}{2}\sigma|\dot{\mathbf{n}}|^2\right\}\mathrm{d}v\leq W(\mathcal{R}(t)), \tag{3.7}$$

with

$$W(\mathcal{R}(t))=\int\limits_{\partial\mathcal{R}(t)}(\mathbf{C}\mathbf{m}_{\partial\mathcal{R}}+\mathbf{q}V^{\mathrm{rel}}_{\partial\mathcal{R}})\cdot\mathbf{v}^{\mathrm{rel}}_{\partial\mathcal{R}}\,\mathrm{d}a+\int\limits_{\partial\mathcal{R}(t)}(\mathbf{S}\mathbf{m}_{\partial\mathcal{R}}+\mathbf{r}V^{\mathrm{rel}}_{\partial\mathcal{R}})\cdot(\dot{\mathbf{n}}+\mathbf{G}\mathbf{v}^{\mathrm{rel}}_{\partial\mathcal{R}})\,\mathrm{d}a$$
$$+\int\limits_{\partial\mathcal{R}(t)}(\mathbf{T}\mathbf{m}_{\partial\mathcal{R}}+\mathbf{p}V^{\mathrm{rel}}_{\partial\mathcal{R}})\cdot\mathbf{v}_{\partial\mathcal{R}}\,\mathrm{d}a \tag{3.8}$$

the power expended by the *effective* standard, director, and configurational tractions on $\partial\mathcal{R}(t)$. Each term of $W(\mathcal{R})$ as defined in (3.8) has a definite physical interpretation:

- Configurational forces are introduced to account for power expenditures associated with material transfer due to the migration of $\partial\mathcal{R}$. Specifically, we view the effective configurational traction $\mathbf{C}\mathbf{m}_{\partial\mathcal{R}}+\mathbf{q}V^{\mathrm{rel}}_{\partial\mathcal{R}}$ as a force, per unit area, associated with the transfer of material across $\partial\mathcal{R}$. Since any velocity field $\mathbf{v}^{\mathrm{rel}}_{\partial\mathcal{R}}$ for $\partial\mathcal{R}$ represents the velocity with which material is transferred across $\partial\mathcal{R}$, we take $\mathbf{v}^{\mathrm{rel}}_{\partial\mathcal{R}}$ to be an appropriate power conjugate velocity for $\mathbf{C}\mathbf{m}_{\partial\mathcal{R}}$. Moreover, material is added to $\mathcal{R}$ only along its boundary $\partial\mathcal{R}$; there is no transfer of material to the interior of $\mathcal{R}$ and, for that reason, the configurational body force density $\mathbf{f}$ expends no power.

- Since $\partial\mathcal{R}$ migrates through the liquid, it has no intrinsic material description. Hence, for the velocity conjugate to the effective standard traction $\mathbf{T}\mathbf{m}_{\partial\mathcal{R}}+\mathbf{p}V^{\mathrm{rel}}_{\partial\mathcal{R}}$, we use, in place of $\mathbf{u}$, the observed velocity $\mathbf{v}_{\partial\mathcal{R}}$ of $\partial\mathcal{R}$.

- Similarly, we assume that the velocity conjugate to the effective director traction $\mathbf{S}\mathbf{m}_{\partial\mathcal{R}}+\mathbf{r}V^{\mathrm{rel}}_{\partial\mathcal{R}}$ is not given by the *material* time derivative $\dot{\mathbf{n}}$ as in the classical theory, but rather by $\dot{\mathbf{n}}+\mathbf{G}\mathbf{v}^{\mathrm{rel}}_{\partial\mathcal{R}}$, the rate of change of the director following the observed motion of $\partial\mathcal{R}$.

By a simple extension of an argument given by Cermelli, Fried & Gurtin [5], we may show that the free-energy inequality in the configurational form (3.7) and subject to the requirement that the power $W(\mathcal{R})$ as defined in (3.8) be independent of the velocity field $\mathbf{v}_{\partial\mathcal{R}}$ chosen to characterize the motion of $\partial\mathcal{R}$ is equivalent to the conventional statement (3.6) of the energy inequality if and only if the configurational momentum $\mathbf{q}$ is related to the standard and director momenta by

$$\mathbf{q}=-(\mathbf{p}+\mathbf{G}^{\top}\mathbf{r})=-\varrho\mathbf{u}-\sigma\mathbf{G}^{\top}\dot{\mathbf{n}} \tag{3.9}$$

and the configurational stress $\mathbf{C}$ is given by the *Eshelby relation*

$$\mathbf{C}=(\Psi-\tfrac{1}{2}\varrho|\mathbf{u}|^2-\tfrac{1}{2}\sigma|\dot{\mathbf{n}}|^2)\mathbf{1}-\mathbf{G}^{\top}\mathbf{S}-\mathbf{T}. \tag{3.10}$$

The argument leading to the relations (3.9) and (3.10) for the configurational momentum and stress make no use of constitutive theory. Hence, in particular, (3.10) applies to broad classes of materials. Moreover, by the momentum balances (2.7), (3.9) and (3.10) yield the result $\dot{\mathbf{q}} - \operatorname{div}\mathbf{C} = \varrho\mathbf{L}^{\top}\mathbf{u} + \sigma\mathbf{G}^{\top}\mathbf{L}\dot{\mathbf{n}} - \operatorname{grad}\Psi + \mathbf{S}\colon\operatorname{grad}\mathbf{G} - \mathbf{G}^{\top}\mathbf{g}$.[5] This result, which is independent of constitution, shows that the internal body force $\mathbf{f}$ in the configurational balance (3.1) has the explicit form

$$\mathbf{f} = \varrho\mathbf{L}^{\top}\mathbf{u} - \operatorname{grad}\Psi + \mathbf{S}\colon\operatorname{grad}\mathbf{G} + \sigma\mathbf{G}^{\top}\mathbf{L}\dot{\mathbf{n}} - \mathbf{G}^{\top}\mathbf{g}. \tag{3.11}$$

Thus, granted (3.9), (3.10), and (3.11), the configurational momentum balance (3.1) is a direct consequence of the momentum balances (2.7).

Using (3.11), the relations (3.9), and (3.10), and the bulk constitutive relations (2.8), we find that the configurational stress $\mathbf{C}$ and internal configurational force $\mathbb{f}$ in the are determined by the fields $\mathbf{u}$, $\mathbf{n}$, and p through the relations

$$\left.\begin{aligned} \mathbf{C} &= (\hat{\Psi}(\mathbf{n},\mathbf{G}) + p - \tfrac{1}{2}\varrho|\mathbf{u}|^2 - \tfrac{1}{2}\sigma|\dot{\mathbf{n}}|^2)\mathbf{1} - \mathbf{T}_{\mathrm{dis}},\\ \mathbf{f} &= \varrho\mathbf{L}^{\top}\mathbf{u} + \sigma\mathbf{G}^{\top}\mathbf{L}\dot{\mathbf{n}} - \mathbf{G}^{\top}\mathbf{g}_{\mathrm{dis}}. \end{aligned}\right\} \tag{3.12}$$

These relations hold regardless of whether $\mathbf{T}_{\mathrm{dis}}$ and $\mathrm{g}_{\mathrm{dis}}$ take the linear forms (2.5). As we will later find, the interfacial counterparts of $\mathbf{C}$ and $\mathbf{f}$, which may be viewed as surface excess quantities, do require independent constitutive specification; moreover, whereas the bulk balance merely determines $\mathbf{f}$, its interfacial counterpart provides an additional evolution equation encompassing the essential physics underlying transitions between the nematic and isotropic phases.

4 Theory for the isotropic phase

We model the isotropic phase as a classical incompressible and viscous liquid. Although the director field and all associated quantities are undefined for such a liquid, we may derive the governing equations for the isotropic phase by formally setting

$$\Psi = 0, \qquad \mathbf{r} = \mathbf{0}, \qquad \mathbf{S} = \mathbf{0}, \qquad \text{and} \qquad \mathbf{g} = \mathbf{0}$$

in the equations for the nematic phase. While the momentum balance is then simply $(2.7)_1$, the angular momentum balance yields in place of (2.9) the usual symmetry relation $\mathbf{T} = \mathbf{T}^{\top}$.

As is conventional, we assume that the Cauchy stress in the isotropic phase is linearly viscous, whereby

$$\mathbf{T} = -p\mathbf{1} + \mathbf{T}_{\mathrm{dis}}, \qquad \mathbf{T}_{\mathrm{dis}} = 2\mu\mathbf{D}, \tag{4.1}$$

with p a constitutively indeterminate pressure and μ the (constant) *shear viscosity*. The governing equations for $\mathbf{u}$ are then the familiar incompressible Navier–Stokes equations

$$\left.\begin{aligned} \operatorname{div}\mathbf{u} &= 0,\\ \varrho\dot{\mathbf{u}} &= -\operatorname{grad}p + \mu\operatorname{div}(\operatorname{grad}\mathbf{u}). \end{aligned}\right\} \tag{4.2}$$

As in the nematic phase, an understanding of the bulk configurational forces in the isotropic phase is superfluous to understanding the flow in that phase but central to the dynamics of the interface. For the isotropic phase, the configurational momentum balance remains (3.1), but now $\mathbf{q}$ and $\mathbf{C}$ are given by

$$\mathbf{q} = -\varrho\mathbf{u} \qquad \text{and} \qquad \mathbf{C} = -\tfrac{1}{2}\varrho|\mathbf{u}|^2\mathbf{1} - \mathbf{T}. \tag{4.3}$$

We therefore have the following isotropic counterpart of (3.12)

$$\mathbf{C} = (p - \tfrac{1}{2}\varrho|\mathbf{u}|^2)\mathbf{1} - 2\mu\mathbf{D}, \qquad \mathbf{f} = \varrho\mathbf{L}^{\top}\mathbf{u}. \tag{4.4}$$

[5] The expression $\mathbf{S}\colon\operatorname{grad}\mathbf{G}$ denotes the vector field defined via the identity $(\mathbf{S}\colon\operatorname{grad}\mathbf{G})\cdot\mathbf{a} = \mathbf{S}\colon\operatorname{grad}(\mathbf{G}\mathbf{a})$ for any constant vector $\mathbf{a}$.

5 Superficial kinematics and basic identities

We suppose that the isotropic and nematic phases are separated by a time-dependent surface $\mathcal{S}$ oriented by a *unit normal field* $\mathtt{m}$, defined over $\mathcal{S}$ for all time, directed from the region occupied by the nematic phase into the region occupied by the isotropic phase.

5.1 Superficial fields

A *superficial field* is a smooth field defined on the interface for all time. A superficial tensor field $\mathbb{A}$ is a tensor field on $\mathcal{S}$ such that $\mathbb{A}\mathtt{m} = \mathbf{0}$.[6] An example of a superficial tensor field is the *projection* onto the tangent space to $\mathcal{S}$

$$\mathbb{P} = \mathbf{1} - \mathtt{m}\otimes\mathtt{m}. \tag{5.1}$$

Each superficial tensor field $\mathbb{A}$ admits a decomposition of the form

$$\mathbb{A} = \mathbb{A}_{\rm tan} + \mathtt{m}\otimes\mathtt{a}, \tag{5.2}$$

in which $\mathbb{A}_{\rm tan} = \mathbb{P}\mathbb{A}$ and $\mathtt{a} = \mathbb{A}^{\top}\mathtt{m}$.

5.2 Superficial gradient and divergence

We denote by $\mathsf{grad}_{\mathcal{S}}$ and $\mathsf{div}_{\mathcal{S}}$ the superficial gradient and divergence. Let $\mathtt{a}$ be a superficial vector field such that $\mathtt{a}\cdot\mathtt{m} = 0$, and let $\mathbb{A}$ be a superficial tensor field. Then the surface divergence theorem asserts that, for any subsurface $\mathcal{A}$ of $\mathcal{S}$,

$$\int\limits_{\partial\mathcal{A}} \mathtt{a}\cdot\mathtt{m}_{\partial\mathcal{A}}\,{\rm d}s = \int\limits_{\partial\mathcal{A}} \mathsf{div}_{\mathcal{S}}\mathtt{a}\,{\rm d}a, \qquad \int\limits_{\partial\mathcal{A}} \mathbb{A}\mathtt{m}_{\partial\mathcal{A}}\,{\rm d}s = \int\limits_{\partial\mathcal{A}} \mathsf{div}_{\mathcal{S}}\mathbb{A}\,{\rm d}a, \tag{5.3}$$

where $\mathtt{m}_{\partial\mathcal{A}}$ is the outward unit normal to $\partial\mathcal{A}$ in the tangent plane to $\mathcal{S}$.

The *curvature tensor* $\mathbb{K}$ defined by

$$\mathbb{K} = -\mathsf{grad}_{\mathcal{S}}\mathtt{m} \tag{5.4}$$

obeys $\mathbb{K}^{\top}\mathtt{m} = \mathbf{0}$ and $\mathbb{K} = \mathbb{K}^{\top}$, and

$$K = \mathsf{tr}\,\mathbb{K} = \mathbb{P}\!:\!\mathbb{K} = -\mathsf{div}_{\mathcal{S}}\mathtt{m} \tag{5.5}$$

is the *total* (twice the mean) *curvature*. Then, by (5.1), we have the important identity

$$\mathsf{div}_{\mathcal{S}}\mathbb{P} = K\mathtt{m}. \tag{5.6}$$

5.3 Superficial limits of bulk fields

Consider an arbitrary bulk field Φ continuous up to $\mathcal{S}$ from either phase. For each $\mathbf{x}$ belonging to $\mathcal{S}(t)$, we denote by Φ^{+} and Φ^{-} the limits $\Phi^{\pm}(\mathbf{x},t) = \lim_{\epsilon\to 0^{+}} \Phi(\mathbf{x}\pm\epsilon\mathtt{m}(\mathbf{x},t),t)$. Further, we use $[\![\Phi]\!]$ and $\langle\!\langle\Phi\rangle\!\rangle$ to designate the *jump* and *average* of Φ across $\mathcal{S}$:

$$[\![\Phi]\!] = \Phi^{+} - \Phi^{-}, \qquad \langle\!\langle\Phi\rangle\!\rangle = \tfrac{1}{2}\big(\Phi^{+} + \Phi^{-}\big).$$

Then, given bulk fields Φ and Λ, we have the useful identity:

$$[\![\Phi\Lambda]\!] = \langle\!\langle\Phi\rangle\!\rangle[\![\Lambda]\!] + \langle\!\langle\Lambda\rangle\!\rangle[\![\Phi]\!]. \tag{5.7}$$

Consider now the fluid velocity field $\mathbf{u}$. We allow for the possibility that the normal components $\mathbf{u}^{\pm}\cdot\mathtt{m}$ of the interfacial limits $\mathbf{u}^{\pm}$ of $\mathbf{u}$ differ.[7] However, we assume that the interface is *slip-free*, i.e.,

$$\mathbb{P}[\![\mathbf{u}]\!] = \mathbf{0} \qquad \Longleftrightarrow \qquad \mathtt{u} := \mathbb{P}\mathbf{u}^{+} = \mathbb{P}\mathbf{u}^{-} = \mathbb{P}\langle\!\langle\mathbf{u}\rangle\!\rangle, \tag{5.8}$$

so that the tangential components $\mathbb{P}\mathbf{u}^{\pm}$ of the interfacial limits $\mathbf{u}^{+}$ and $\mathbf{u}^{-}$ of $\mathbf{u}$ coincide.

[6] A superficial tensor field would generally be defined at each $\mathbf{x}\in\mathcal{S}$ as a linear transformation of the tangent space at $\mathbf{x}$ into $\mathbb{R}^3$; the requirement $\mathbb{A}\mathtt{m} = \mathbf{0}$ allows us to consider $\mathbb{A}$ at each point as a linear transformation of $\mathbb{R}^3$ into $\mathbb{R}^3$.

[7] By the interfacial mass balance (6.1), the fluid velocity must be discontinuous across $\mathcal{S}$ whenever the densities of the nematic and isotropic phases differ.

5.4 Velocity fields for $\mathcal{S}$

Let $\mathtt{v}$ denote a *velocity field* for $\mathcal{S}$. The tangential component of a velocity field for $\mathcal{S}$ can be chosen arbitrarily, since it corresponds to a choice of parametrization of $\mathcal{S}$, but all velocity fields must have the same normal component

$$V := \mathtt{v}\cdot\mathtt{m},$$

which we refer to as the *normal velocity of the interface*. The fields

$$\mathtt{v} - \mathbf{u}^{\pm} \qquad \text{and} \qquad V - \mathbf{u}^{\pm}\cdot\mathtt{m}$$

represent vector and scalar velocities of $\mathcal{S}$ relative to the isotropic and nematic phases.

Consider an arbitrary subsurface $\mathcal{A}$ of $\mathcal{S}$. The curve $\partial\mathcal{A}$ evolves in space and its motion is described by a velocity field $\mathtt{v}_{\partial\mathcal{A}}$ on $\partial\mathcal{A}$. Different parametrizations of the curve $\partial\mathcal{A}$ induce different velocity fields, but all velocity fields must have the same components V and $V_{\partial\mathcal{A}}$ with respect to the unit normals $\mathtt{m}$ and $\mathtt{m}_{\partial\mathcal{A}}$, i.e.,

$$\mathtt{v}_{\partial\mathcal{A}}\cdot\mathtt{m} = V \qquad \text{and} \qquad \mathtt{v}_{\partial\mathcal{A}}\cdot\mathtt{m}_{\partial\mathcal{A}} = V_{\partial\mathcal{A}}. \tag{5.9}$$

The motion of $\partial\mathcal{A}$ relative to the material in the bulk phases is then described by the relative velocities

$$\mathtt{v}_{\partial\mathcal{A}} - \mathbf{u}^{\pm} \qquad \text{and} \qquad V_{\partial\mathcal{A}} - \mathtt{u}\cdot\mathtt{m}_{\partial\mathcal{A}}. \tag{5.10}$$

The component of $\mathtt{v}_{\partial\mathcal{A}}$ tangential to $\partial\mathcal{A}$ is not intrinsic and *may be arbitrarily chosen*. We require that the theory not depend on the velocity field $\mathtt{v}_{\partial\mathcal{A}}$ chosen to characterize the migration of $\partial\mathcal{A}$, and therefore that the theory be invariant under transformations of $\mathtt{v}_{\partial\mathcal{A}}$ of the form

$$\mathtt{v}_{\partial\mathcal{A}} \to \mathtt{v}_{\partial\mathcal{A}} + \mathtt{t}, \tag{5.11}$$

with $\mathtt{t}$ tangent to $\partial\mathcal{A}$.

5.5 Materially intrinsic velocity field for $\mathcal{S}$

To formulateintegral laws for an interface $\mathcal{S}$ migrating through the fluid, what is needed is a velocity field for $\mathcal{S}$ that characterizes its *migration*. Specifically, we seek a single velocity field $\mathtt{v}$ for $\mathcal{S}$ that renders each of the migrational velocities $\mathtt{v} - \mathbf{u}^{\pm}$ normal. With this in mind, we note that

$$\mathtt{v} - \mathbf{u}^{\pm} = \mathtt{v} - (\mathbf{u}^{\pm}\cdot\mathbf{n})\mathtt{m} - \mathtt{u} = (V - \mathbf{u}^{\pm}\cdot\mathbf{n})\mathbf{n} + (\mathbb{P}\mathtt{v} - \mathtt{u});$$

thus, taking $\mathbb{P}\mathtt{v} = \mathtt{u}$, we arrive at a choice of velocity field $\mathtt{v}$ for $\mathcal{S}$ with each of its migrational velocities $\mathtt{v} - \mathbf{u}^{\pm}$ normal:

$$\mathtt{v} - \mathbf{u}^{\pm} = (V - \mathbf{u}^{\pm}\cdot\mathtt{m})\mathtt{m}. \tag{5.12}$$

Since $\mathbf{u}^{\pm} - (\mathbf{u}^{\pm}\cdot\mathbf{n})\mathtt{m} = \mathtt{u}$, the resulting velocity field $\mathtt{v}$, called the *materially intrinsic velocity-field* for $\mathcal{S}$, has the specific form

$$\mathtt{v} = V\mathtt{m} + \mathtt{u} \tag{5.13}$$

and is important *because it is normal when computed relative to the material on either side of* $\mathcal{S}(t)$.

For $\mathtt{v}$ the materially intrinsic velocity-field for $\mathcal{S}$, the migrational velocity $\mathtt{v} - \langle\!\langle\mathbf{u}\rangle\!\rangle$ satisfies

$$\mathtt{v} - \langle\!\langle\mathbf{u}\rangle\!\rangle = (V - \langle\!\langle\mathbf{u}\rangle\!\rangle\cdot\mathbf{n})\mathtt{m}. \tag{5.14}$$

Similarly, by (5.9), (5.10), and (5.12), we also have the identity

$$\begin{aligned}(\mathtt{v}_{\partial\mathcal{A}} - \mathtt{v})\cdot\mathtt{m}_{\partial\mathcal{A}} &= (\mathtt{v}_{\partial\mathcal{A}} - \mathbf{u}^{\pm})\cdot\mathtt{m}_{\partial\mathcal{A}} - (\mathtt{v} - \mathbf{u}^{\pm})\cdot\mathtt{m}_{\partial\mathcal{A}}\\ &= V_{\partial\mathcal{A}} - \mathtt{u}\cdot\mathtt{m}_{\partial\mathcal{A}}.\end{aligned} \tag{5.15}$$

Further, in view of $(5.4)_1$ and (5.13),

$$\mathsf{grad}_{\mathcal{S}}\mathtt{v} = \mathtt{m}\otimes\mathsf{grad}_{\mathcal{S}}V - V\mathbb{K} + \mathsf{grad}_{\mathcal{S}}\mathtt{u}. \tag{5.16}$$

5.6 Materially intrinsic time-derivative. Superficial transport theorem

Let γ be a field on $\mathcal{S}$ and let $\mathtt{v}$ be the materially intrinsic velocity field for $\mathcal{S}$ (cf. (5.13)). Given any time t_0 and any point $\mathbf{x}_0$ on $\mathcal{S}(t_0)$, let $\mathbf{z}(t)$ denote the curve such that

$$\frac{\mathrm{d}\mathbf{z}(t)}{\mathrm{d}t} = \mathtt{v}(\mathbf{z}(t),t), \qquad \mathbf{z}(t_0) = \mathbf{x}_0,$$

and define

$$\mathring{\gamma}(\mathbf{x}_0,t_0) = \left.\frac{\mathrm{d}\gamma(\mathbf{z}(t),t)}{\mathrm{d}t}\right|_{t=t_0}. \tag{5.17}$$

The field $\mathring{\gamma}$ defined in this manner is referred to as the *materially intrinsic normal time-derivative of* γ *following* $\mathcal{S}$.

Important to what follows is the *superficial transport theorem* (Cermelli, Fried & Gurtin [6]): for $\gamma(\mathbf{x},t)$ a smooth superficial scalar field,

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{A}} \gamma\,\mathrm{d}a = \int_{\mathcal{A}} \Big\{\mathring{\gamma} - \gamma\,(KV - \mathsf{div}_{\mathcal{S}}\mathtt{u})\Big\}\,\mathrm{d}a + \int_{\partial\mathcal{A}} \gamma(V_{\partial\mathcal{A}} - \mathtt{u}\cdot\mathtt{m}_{\partial\mathcal{A}})\,\mathrm{d}s. \tag{5.18}$$

5.7 Superficial velocity gradient

We write

$$\mathbb{L} = \mathsf{grad}_{\mathcal{S}}\langle\!\langle\mathbf{u}\rangle\!\rangle = \langle\!\langle\mathbf{L}\rangle\!\rangle\mathbb{P} \tag{5.19}$$

for the *superficial velocity gradient* and define the *superficial rate of stretch* $\mathbb{D}$ and the *superficial rate of spin* $\mathbb{W}$ via

$$\mathbb{D} = \tfrac{1}{2}(\mathbb{P}\mathbb{L} + \mathbb{L}^{\top}\mathbb{P}) = \mathbb{P}\langle\!\langle\mathbf{D}\rangle\!\rangle\mathbb{P}, \qquad \mathbb{W} = \tfrac{1}{2}(\mathbb{P}\mathbb{L} - \mathbb{L}^{\top}\mathbb{P}) = \mathbb{P}\langle\!\langle\mathbf{W}\rangle\!\rangle\mathbb{P}. \tag{5.20}$$

Then $\mathbb{L} = \mathbb{D} + \mathbb{W} + \mathtt{m}\otimes\mathbb{L}^{\top}\mathtt{m}$ and, for any superficial tensor field $\mathbb{A}$,

$$\mathbb{A}\!:\!\mathbb{L} = \mathbb{A}_{\tan}\!:\!(\mathbb{D}+\mathbb{W}) + \mathbb{A}^{\top}\mathtt{m}\cdot\mathbb{L}^{\top}\mathtt{m}. \tag{5.21}$$

In the subsequent development we will require a measure of the rate of change of the director field following the interface. A natural choice for such a measure would appear to be $\mathring{\mathbf{n}}$; however, $\mathring{\mathbf{n}}$ is not invariant under superimposed rigid-body motions. Among all possible properly invariant choices, we will use the superficial field

$$\mathtt{w} = \mathring{\mathbf{n}} - \mathbb{W}\mathbf{n} + (\mathbf{n}\cdot\mathtt{m})\mathbb{L}^{\top}\mathtt{m} - (\mathbf{n}\cdot\mathbb{L}^{\top}\mathtt{m})\mathtt{m}, \tag{5.22}$$

which obeys $\mathtt{w}\cdot\mathbf{n} = 0$. Thus, introducing

$$\xi = \mathbf{n}\cdot\mathtt{m} \tag{5.23}$$

and noting that $\mathring{\mathbf{n}}\cdot\mathtt{m} = \mathtt{w}\cdot\mathtt{m} + \mathbf{n}\cdot\mathbb{L}^{\top}\mathtt{m}$, $\mathring{\mathtt{m}}\cdot\mathbf{n} = -\mathbf{n}\cdot\mathsf{grad}_{\mathcal{S}}(V - \langle\!\langle\mathbf{u}\rangle\!\rangle\cdot\mathtt{m}) - \mathbf{n}\cdot\mathbb{L}^{\top}\mathtt{m} - \mathbf{n}\cdot\mathbb{K}(\mathtt{v} - \langle\!\langle\mathbf{u}\rangle\!\rangle)$, $\mathtt{m}\cdot\mathtt{w} = (\mathtt{m} - \xi\mathbf{n})\cdot\mathtt{w}$, and $\mathbf{n}\cdot\mathsf{grad}_{\mathcal{S}}J = (\mathbf{n} - \xi\mathtt{m})\cdot\mathsf{grad}_{\mathcal{S}}J$, it follows that

$$\mathring{\xi} = (\mathtt{m} - \xi\mathbf{n})\cdot\mathtt{w} - \langle\!\langle\upsilon\rangle\!\rangle(\mathbf{n} - \xi)\cdot\mathsf{grad}_{\mathcal{S}}J - \mathbf{n}\cdot\mathbb{K}(\mathtt{v} - \langle\!\langle\mathbf{u}\rangle\!\rangle)$$

and thus, by (5.14), that for $\mathtt{v}$ materially intrinsic,

$$\mathring{\xi} = (\mathtt{m} - \xi\mathbf{n})\cdot\mathtt{w} - \langle\!\langle\upsilon\rangle\!\rangle(\mathbf{n} - \xi\mathtt{m})\cdot\mathsf{grad}_{\mathcal{S}}J. \tag{5.24}$$

6 Superficial kinetics

6.1 Pillboxes

Let $\mathcal{A}$ be an arbitrary subsurface of $\mathcal{S}$. The *superficial pillbox* determined by $\mathcal{A}$ is a control volume of infinitesimal thickness consisting of (Fig. 1):

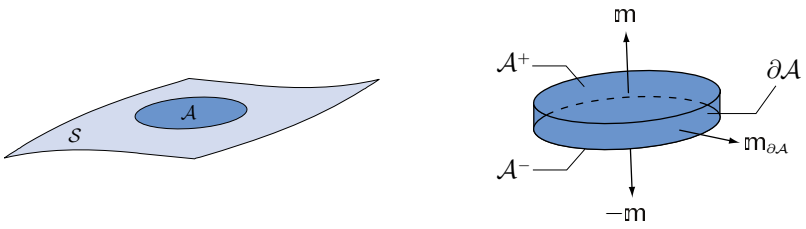

Figure 1: Schematic of a migrating subsurface $\mathcal{A}$ of the interface $\mathcal{S}$ showing an enlarged view of the associated superficial pillbox.

- a surface $\mathcal{A}^+$, with unit normal $\mathbb{m}$, lying in the isotropic phase;
- a surface $\mathcal{A}^-$, with unit normal $-\mathbb{m}$, lying in the nematic phase;
- a lateral bounding surface $\partial\mathcal{A}$ with outward unit normal $\mathbb{m}_{\partial\mathcal{A}}$.

To write the basic laws for an interfacial pillbox, consider a typical balance in integral form for a time-dependent control volume $\mathcal{R}$ defined so that $\mathcal{A} = \mathcal{R} \cap \mathcal{S}$:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{R}} \mathbf{a}\,\mathrm{d}v = \int_{\partial\mathcal{R}} \left\{\mathbf{A}\mathbf{m}_{\partial\mathcal{R}} + \mathbf{a}V^{\mathrm{rel}}_{\partial\mathcal{R}}\right\}\mathrm{d}a + \int_{\mathcal{R}} \mathbf{b}\,\mathrm{d}v + \left\{\begin{array}{c}\text{interfacial}\\ \text{terms}\end{array}\right\},$$

with $\mathbf{a}$ and $\mathbf{b}$ vector fields, $\mathbf{A}$ a tensor field, and $\mathbf{m}_{\partial\mathcal{R}}$ the outward unit normal to $\partial\mathcal{R}$. If these fields admit limit and are smooth up to the interface, standard arguments show that this balance implies a corresponding integral balance

$$\int_{\mathcal{A}} [\![\mathbf{A}\mathbb{m} + (V - \mathbf{u}\cdot\mathbb{m})\mathbf{a}]\!]\,\mathrm{d}a + \left\{\begin{array}{c}\text{interfacial}\\ \text{terms}\end{array}\right\} = \mathbf{0},$$

for $\mathcal{A}$.

6.2 Mass balance

The isotropic and nematic phases are endowed with constant mass densities ϱ^+ and ϱ^-. We allow for the possibility that these densities differ. The fields $\varrho^\pm(V - \mathbf{u}^\pm\cdot\mathbb{m})$ then represent flows of mass at the two sides of the interface in the direction $\mathbb{m}$, and balance of mass requires that these be equal:

$$[\![\varrho(V - \mathbf{u}\cdot\mathbb{m})]\!] = 0. \tag{6.1}$$

Thus, we may define the *mass flow* J across the interface (in the direction $\mathbf{n}$) by the relation

$$J = \varrho^+(V - \mathbf{u}^+\cdot\mathbb{m}) = \varrho^-(V - \mathbf{u}^-\cdot\mathbb{m}), \tag{6.2}$$

so that

$$J = \langle\!\langle v\rangle\!\rangle^{-1}(V - \langle\!\langle\mathbf{u}\rangle\!\rangle\cdot\mathbb{m}) \qquad \text{and} \qquad [\![v]\!]J = -[\![\mathbf{u}]\!]\cdot\mathbb{m}, \tag{6.3}$$

with

$$v = \frac{1}{\varrho}$$

the *specific volume*.

6.3 Balance of linear momentum

In addition to the bulk Cauchy stress, we account for *interfacial Cauchy stress* through a superficial tensor field $\mathbb{T}$. The balance of linear momentum for a superficial pillbox $\mathcal{A}$ then requires that

$$\int_{\partial\mathcal{A}} \mathbb{T}\,\mathbb{m}_{\partial\mathcal{A}}\,\mathrm{d}s + \int_{\mathcal{A}} \left\{[\![\mathbf{T}]\!]\mathbb{m} + [\![(V - \mathbf{u}\cdot\mathbb{m})\mathbf{p}]\!]\right\}\mathrm{d}a = \mathbf{0},$$

or, equivalently, that the superficial field equation

$$\mathsf{div}_{\mathcal{S}}\mathbb{T} + [\![\mathbf{T}]\!]\mathbb{m} + [\![(V - \mathbf{u}\cdot\mathbb{m})\mathbf{p}]\!] = \mathbf{0} \tag{6.4}$$

holds on $\mathcal{S}$.

6.4 Balance of director momentum

In addition to the bulk director stress $\mathbf{S}$ and the bulk internal director body force $\mathbf{g}$, we account for a *superficial director force* (density) through a field $\mathbf{g}$. The balance of director momentum then requires that, for any superficial pillbox $\mathcal{A}$,

$$\int_{\mathcal{A}} \Big\{\mathbf{g} - \mathbf{S}\mathbb{m} - (V - \mathbf{u}^{-}\cdot\mathbb{m})\mathbf{r}\Big\}\,\mathrm{d}a = \mathbf{0}$$

or, equivalently, that the superficial field equation

$$\mathbf{g} = \mathbf{S}\mathbb{m} + (V - \mathbf{u}^{-}\cdot\mathbb{m})\mathbf{r} \tag{6.5}$$

holds on $\mathcal{S}$. As with its bulk counterpart $(2.7)_2$, we may decompose the interfacial director momentum balance into components

$$(\mathbf{1} - \mathbf{n}\otimes\mathbf{n})(\mathbf{g} - \mathbf{S}\mathbb{m}) = (V - \mathbf{u}^{-}\cdot\mathbb{m})\mathbf{r} \tag{6.6}$$

and

$$\mathbf{g}\cdot\mathbf{n} = (\mathbf{S}^{\top}\mathbf{n})\cdot\mathbb{m} \tag{6.7}$$

perpendicular and parallel to the director.

By $(2.8)_2$ and the requirement that $(\partial\Psi/\partial\mathbf{G})^{\top}\mathbf{n} = \mathbf{0}$, (6.7) yields

$$\mathbf{g}\cdot\mathbf{n} = \boldsymbol{\alpha}\cdot\mathbb{m}, \tag{6.8}$$

so that the component of $\mathbf{g}$ parallel to $\mathbf{n}$ is determined by the multiplier field $\boldsymbol{\alpha}$ and the orientation $\mathbb{m}$ of $\mathcal{S}$. Further, by $(2.8)_2$, (6.6) can be written as

$$(\mathbf{1} - \mathbf{n}\otimes\mathbf{n})\mathbf{g} = \frac{\partial\Psi}{\partial\mathbf{G}}\mathbb{m} + (V - \mathbf{u}^{-}\cdot\mathbb{m})\mathbf{r}, \tag{6.9}$$

showing that only the component of $\mathbf{g}$ parallel to $\mathbf{n}$ is determined in terms of $\boldsymbol{\alpha}$.

6.5 Balance of angular momentum

The balance of angular momentum requires that, for any superficial pillbox $\mathcal{A}$ and any element $\mathbf{o}$ of $\mathbb{R}^3$,

$$\int_{\partial\mathcal{A}} (\mathbf{x} - \mathbf{o})\times\mathbb{T}\mathbb{m}_{\partial\mathcal{A}}\,\mathrm{d}s + \int_{\mathcal{A}} (\mathbf{x} - \mathbf{o})\times\Big\{[\![\mathbf{T}]\!]\mathbb{m} + [\![(V - \mathbf{u}\cdot\mathbb{m})\mathbf{p}]\!]\Big\}\,\mathrm{d}a - \int_{\mathcal{A}} \mathbf{n}\times\Big\{\mathbf{S}\mathbb{m} + (V - \mathbf{u}^{-}\cdot\mathbb{m})\mathbf{r}\Big\}\,\mathrm{d}a = \mathbf{0}$$

or, equivalently, using (6.4) and (6.9), that the superficial field equation

$$\mathbb{T} + \mathbf{n}\otimes\mathbf{g} = (\mathbb{T} + \mathbf{n}\otimes\mathbf{g})^{\top}, \tag{6.10}$$

holds on $\mathcal{S}$. The requirement (6.10) is analogous to the local statement (2.9) of angular momentum balance in the nematic phase. Since $\mathbb{T}$ is a superficial tensor field, $\mathbb{T}\mathbb{m} = \mathbf{0}$ and it follows from (6.10) that

$$\left.\begin{aligned} \mathbb{T}^{\top}\mathbb{m} &= (\mathbf{g}\cdot\mathbb{m})\mathbf{n} - \xi\mathbf{g}, \\ \mathrm{Skw}(\mathbb{T}_{\tan}) &= \tfrac{1}{2}\mathbb{P}(\mathbf{g}\otimes\mathbf{n} - \mathbf{n}\otimes\mathbf{g})\mathbb{P}. \end{aligned}\right\} \tag{6.11}$$

6.6 Balance of configurational momentum

In addition to the bulk configurational stress tensor $\mathbf{C}$ and the bulk internal configurational body force $\mathbf{f}$, we account for *superficial configurational stress* and *superficial internal configurational body force* (*density*) through fields $\mathbb{C}$ and $\mathtt{f}$. The balance of configurational momentum then requires that, for any superficial pillbox $\mathcal{A}$,

$$\int\limits_{\partial\mathcal{A}} \mathbb{C}\mathtt{m}_{\partial\mathcal{A}}\,\mathrm{d}s + \int\limits_{\mathcal{A}} \Big\{\mathtt{f} + [\![\mathbf{C}]\!]\mathtt{m} + [\![(V-\mathbf{u}\cdot\mathtt{m})\mathbf{q}]\!]\Big\}\,\mathrm{d}a = \mathbf{0}$$

or, equivalently, that the superifical field equation

$$\mathsf{div}_{\mathcal{S}}\mathbb{C} + \mathtt{f} + [\![\mathbf{C}]\!]\mathtt{m} + [\![(V-\mathbf{u}\cdot\mathtt{m})\mathbf{q}]\!] = \mathbf{0} \tag{6.12}$$

holds on $\mathcal{S}$.

The role of the interfacial configurational force $\mathtt{f}$ here is completely different from its bulk counterpart $\mathbf{f}$. While $\mathbf{f}$ is indeterminate, and must be chosen so that the bulk equation (3.1) is identically satisfied, $\mathtt{f}$ is in general given by constitutive relations describing the ordering kinetics at the phase interface, and this in turn leads from (6.12) an evolution equation for the interface.

6.7 Power

To express the power expended by the tractions, we mimick the reasoning underlying the form (3.8) of the power expenditure on a control volume migrating through the nematic phase. The configurational and standard tractions $\mathbb{C}\mathtt{m}_{\partial\mathcal{A}}$ and $\mathbb{T}\mathtt{m}_{\partial\mathcal{A}}$ are distributed over the boundary $\partial\mathcal{A}$ of the pillbox. As in our discussion of the bulk phases, we take the migrational velocity $\mathtt{v}_{\partial\mathcal{A}} - \langle\!\langle\mathbf{u}\rangle\!\rangle$ of $\partial\mathcal{A}$ to be the appropriate power conjugate velocity for $\mathbb{C}\mathtt{m}_{\partial\mathcal{A}}$. For $\mathbb{T}\mathtt{m}_{\partial\mathcal{A}}$, we reason by analogy to our treatment of the power expended by the standard traction on a migrating control volume and take as power conjugate the observed velocity $\mathtt{v}_{\partial\mathcal{A}}$ of $\partial\mathcal{A}$. In addition, we view the configurational tractions $\mathbf{C}^{+}\mathtt{m}$ and $-\mathbf{C}^{-}\mathtt{m}$ exerted on $\mathcal{A}$ by the bulk material in the isotropic and nematic phases as forces, per unit area, associated with the transfer of material across $\mathcal{S}$ that occurs with as one phase grows with respect to the other. We therefore take the velocities $\mathtt{v}-\mathbf{u}^{\pm}$ of $\mathcal{S}$ relative to the underlying material to be appropriate power conjugate velocities for $(\mathbf{C}\mathtt{m}+(V-\mathbf{u}\cdot\mathtt{m})\mathbf{q})^{\pm}$. Consistent with our treatment of the power expended by the standard traction on a migrating control volume, we use as a power conjugate velocity for $(\mathbf{T}\mathtt{m}+(V-\mathbf{u}\cdot\mathtt{m})\mathbf{p})^{\pm}$ the velocity $\mathtt{v}$ of $\mathcal{S}$. Similarly, consistent with our treatment of the power expendend by the director traction on a migrating control volume, we use as a power conjugate velocity for $\mathbf{S}\mathtt{m}+(V-\mathbf{u}^{-}\cdot\mathtt{m})\mathbf{r}$ the velocity $\overset{\circ}{\mathbf{n}}$. The (net) external power expended on $\mathcal{A}$ then has the form

$$w(\mathcal{A}) = w^{*}(\mathcal{A}) + \int\limits_{\mathcal{A}} [\![\mathbf{T}\mathtt{m}+(V-\mathbf{u}\cdot\mathtt{m})\mathbf{p}]\!]\cdot\mathtt{v}\,\mathrm{d}a - \int\limits_{\mathcal{A}} \mathtt{g}\cdot\overset{\circ}{\mathbf{n}}\,\mathrm{d}a + \int\limits_{\mathcal{A}} \Big[\![(\mathbf{C}\mathtt{m}+(V-\mathbf{u}\cdot\mathtt{m})\mathbf{q})\cdot(\mathtt{v}-\mathbf{u})]\!]\Big\}\,\mathrm{d}a, \tag{6.13}$$

where we have used the superficial director momentum balance (6.5) and $w^{*}(\mathcal{A})$ is defined by

$$w^{*}(\mathcal{A}) = \int\limits_{\partial\mathcal{A}} \Big\{\mathbb{T}\mathtt{m}_{\partial\mathcal{A}}\cdot\mathtt{v}_{\partial\mathcal{A}} + \mathbb{C}\mathtt{m}_{\partial\mathcal{A}}\cdot(\mathtt{v}_{\partial\mathcal{A}} - \langle\!\langle\mathbf{u}\rangle\!\rangle)\Big\}\,\mathrm{d}s.$$

As in our treatment of the power acting on a migrating control volume, we require that (6.13) be independent of the choice of observed velocity field $\mathtt{v}_{\partial\mathcal{A}}$ chosen to characterize the migration of $\mathcal{A}$. Necessary and sufficient for this condition to be satisfied is that $w^{*}(\mathcal{A})$ be invariant under all transformations of the form

$$\mathtt{v}_{\partial\mathcal{A}} \mapsto \mathtt{v}_{\partial\mathcal{A}} + \mathtt{t}, \qquad \mathtt{t}\cdot\mathtt{m} = \mathtt{t}\cdot\mathtt{m}_{\partial\mathcal{A}} = 0, \tag{6.14}$$

which, by (5.10), is necessarily accompanied by the transformation

$$\mathtt{v}_{\partial\mathcal{A}} - \langle\!\langle\mathbf{u}\rangle\!\rangle \mapsto \mathtt{v}_{\partial\mathcal{A}} - \langle\!\langle\mathbf{u}\rangle\!\rangle + \mathtt{t}, \tag{6.15}$$

This invariance holds if and only if

$$\int\limits_{\mathcal{A}} (\mathbb{T}+\mathbb{C})\mathtt{m}_{\partial\mathcal{A}}\cdot\mathtt{t}\,\mathrm{d}s = 0 \tag{6.16}$$

for all subsurfaces $\mathcal{A}$ of $\mathcal{S}$ and all fields $\mathtt{t}$ tangential to $\partial\mathcal{A}$. It follows that $\mathbb{A} = \mathbb{T} + \mathbb{C}$ must satisfy

$$\mathtt{t}\cdot\mathbb{A}\mathtt{m}^{\perp} = 0 \tag{6.17}$$

whenever $\mathtt{t}$ and $\mathtt{m}^{\perp}$ are orthogonal and tangent to $\mathcal{S}$. Thus $\mathbb{A}\mathtt{m}^{\perp}$ must lie in the direction of $\mathtt{m}^{\perp}$ for each $\mathtt{m}^{\perp}$ orthogonal to $\mathtt{m}$, which is possible if and only if the tangential component $\mathbb{A}_{\rm tan}$ of $\mathbb{A}$ has the form $\mathbb{A}_{\rm tan} = \varphi\mathbb{P}$, with φ a superficial scalar field. Invariance therefore implies that the tangential component $\mathbb{C}_{\rm tan}$ of interfacial configurational stress $\mathbb{C}$ must be of the form

$$\mathbb{C}_{\rm tan} = \varphi\,\mathbb{P} - \mathbb{T}_{\rm tan}. \tag{6.18}$$

We view (6.18) as a *superficial pre-Eshelby relation*. Equivalently, bearing in mind (5.2), we have that

$$\mathbb{C} = \varphi\mathbb{P} - \mathbb{T} + \mathtt{m}\otimes\mathtt{k}, \tag{6.19}$$

with

$$\mathtt{k} = (\mathbb{C} + \mathbb{T})^{\top}\mathtt{m} \tag{6.20}$$

the (*effective*) *configurational shear*.

By (5.15) and (6.18), it follows that

$$w^*(\mathcal{A}) = \int\limits_{\partial\mathcal{A}} \Big\{\varphi(V_{\partial\mathcal{A}} - \mathtt{u}\cdot\mathtt{m}_{\partial\mathcal{A}}) + \mathbb{T}\mathtt{m}_{\partial\mathcal{A}}\cdot\mathtt{v} + \mathbb{C}\mathtt{m}_{\partial\mathcal{A}}\cdot(\mathtt{v} - \langle\!\langle\mathbf{u}\rangle\!\rangle)\Big\}\,{\rm d}s.$$

Further, using the surface divergence theorem $(5.3)_3$ and the superficial balances (6.4) and (6.12) for standard and configurational momentum, we obtain

$$\begin{aligned} w^*(\mathcal{A}) = \int\limits_{\partial\mathcal{A}} \varphi(V_{\partial\mathcal{A}} - \mathtt{u}\cdot\mathtt{m}_{\partial\mathcal{A}})\,{\rm d}s + \int\limits_{\mathcal{A}} \Big\{\mathbb{T}\,\vdots\,\mathsf{grad}_{\mathcal{S}}\mathtt{v} + \mathbb{C}\,\vdots\,\mathsf{grad}_{\mathcal{S}}(\mathtt{v} - \langle\!\langle\mathbf{u}\rangle\!\rangle)\Big\}\,{\rm d}a \\ - \int\limits_{\mathcal{A}} [\![\mathbf{T}\mathtt{m} + (V - \mathbf{u}\cdot\mathtt{m})\mathbf{p}]\!]\cdot\mathtt{v}\,{\rm d}a + \int\limits_{\mathcal{A}} \Big\{\mathtt{f} + [\![\mathbf{C}\mathtt{m} + (V - \mathbf{u}\cdot\mathtt{m})\mathbf{q}]\!]\Big\}\cdot(\mathtt{v} - \langle\!\langle\mathbf{u}\rangle\!\rangle)\,{\rm d}a \end{aligned}$$

and, thus, using (5.7) and recalling that $\mathtt{v}$ is a superficial field to yield

$$\begin{aligned} [\![\mathbf{C}\mathtt{m} + (V - \mathbf{u}\cdot\mathtt{m})\mathbf{q}]\!]\cdot(\mathtt{v} - \langle\!\langle\mathbf{u}\rangle\!\rangle) &= [\![\mathbf{C}\mathtt{m} + (V - \mathbf{u}\cdot\mathtt{m})\mathbf{q}\cdot(\mathtt{v} - \mathbf{u})]\!] - \langle\!\langle\mathbf{C}\mathtt{m} + (V - \mathbf{u}\cdot\mathtt{m})\mathbf{q}\rangle\!\rangle\cdot[\![\mathtt{v} - \mathbf{u}]\!] \\ &= [\![\mathbf{C}\mathtt{m} + (V - \mathbf{u}\cdot\mathtt{m})\mathbf{q}\cdot(\mathtt{v} - \mathbf{u})]\!] + \langle\!\langle\mathbf{C}\mathtt{m} + (V - \mathbf{u}\cdot\mathtt{m})\mathbf{q}\rangle\!\rangle\cdot[\![\mathbf{u}]\!], \end{aligned}$$

find that (6.13) can be expressed as

$$\begin{aligned} w(\mathcal{A}) = \int\limits_{\partial\mathcal{A}} \varphi(V_{\partial\mathcal{A}} - \mathtt{u}\cdot\mathtt{m}_{\partial\mathcal{A}})\,{\rm d}s + \int\limits_{\mathcal{A}} \Big\{(\mathbb{T} + \mathbb{C})\,\vdots\,\mathsf{grad}_{\mathcal{S}}\mathtt{v} - \mathbb{C}\,\vdots\,\mathbb{L} - \mathtt{g}\cdot\mathring{\mathbf{n}}\Big\}\,{\rm d}a \\ - \int\limits_{\mathcal{A}} \Big\{\mathtt{f}\cdot(\mathtt{v} - \langle\!\langle\mathbf{u}\rangle\!\rangle) + \langle\!\langle\mathbf{C}\mathtt{m} + (V - \mathbf{u}\cdot\mathtt{m})\mathbf{q}\rangle\!\rangle\cdot[\![\mathbf{u}]\!]\Big\}\,{\rm d}a. \end{aligned} \tag{6.21}$$

Toward a further simplification of the expression for the total power expended on $\mathcal{A}$, consider the second term on the right side of (6.21). By (6.19),

$$\begin{aligned} (\mathbb{T} + \mathbb{C})\,\vdots\,\mathsf{grad}_{\mathcal{S}}\mathtt{v} &= \Big\{(\mathbb{T} + \mathbb{C})_{\rm tan} + \mathtt{m}\otimes\mathtt{k}\Big\}\,\vdots\,\mathsf{grad}_{\mathcal{S}}\mathtt{v} \\ &= \varphi\mathsf{div}_{\mathcal{S}}\mathtt{v} + (\mathtt{m}\otimes\mathtt{k})\,\vdots\,\mathsf{grad}_{\mathcal{S}}\mathtt{v}. \end{aligned}$$

Also, by (5.19), (5.21), (6.11), (6.20), and (6.19),

$$\begin{aligned} \mathbb{C}\,\vdots\,\mathbb{L} &= \mathbb{C}_{\rm tan}\,\vdots\,(\mathbb{D} + \mathbb{W}) + \mathbb{C}^{\top}\mathtt{m}\cdot\mathbb{L}^{\top}\mathtt{m} + \mathtt{g}\cdot\mathring{\mathbf{n}} \\ &= \mathbb{C}_{\rm tan}\,\vdots\,\mathbb{D} - \mathbb{T}_{\rm tan}\,\vdots\,\mathbb{W} + (\mathtt{k} - \mathbb{T}^{\top}\mathtt{m})\cdot\mathbb{L}^{\top}\mathtt{m} + \mathtt{g}\cdot\mathring{\mathbf{n}} \\ &= \mathbb{C}_{\rm tan}\,\vdots\,\mathbb{D} + (\mathtt{m}\otimes\mathtt{k})\,\vdots\,\mathbb{L} + \mathtt{g}\cdot\mathtt{w}. \end{aligned}$$

Thus,

$$(\mathbb{T}+\mathbb{C})\colon \mathsf{grad}_s \mathbb{v} - \mathbb{C}\colon \mathbb{L} - \mathbb{g}\cdot\mathring{\mathbb{n}} = \varphi \mathsf{div}_s \mathbb{v} - \mathbb{C}_{\tan}\colon \mathbb{D} - \mathbb{g}\cdot\mathbb{w} + (\mathbb{m}\otimes\mathbb{k})\colon \mathsf{grad}_s(\mathbb{v} - \langle\!\langle \mathbf{u} \rangle\!\rangle), \tag{6.22}$$

Hereafter, we require that the velocity field $\mathbb{v}$ for $\mathcal{S}$ be migrationally intrinsic. In view of (5.14), (5.16), and (6.3), we may therefore rewrite (6.22) in the form

$$(\mathbb{T}+\mathbb{C})\colon \mathsf{grad}_s \mathbb{v} - \mathbb{C}\colon \mathbb{L} - \mathbb{g}\cdot\mathring{\mathbb{n}} = -\varphi(KV - \mathsf{div}_s \mathbb{u}) - \mathbb{C}_{\tan}\colon \mathbb{D} - \mathbb{g}\cdot\mathbb{w} + \langle\!\langle \upsilon \rangle\!\rangle \mathbb{k}\cdot\mathsf{grad}_s J, \tag{6.23}$$

Next, consider the final term on the right side of (6.21). By $(6.3)_1$ and (5.14),

$$\mathbb{f}\cdot(\mathbb{v} - \langle\!\langle \mathbf{u} \rangle\!\rangle) = \langle\!\langle \upsilon \rangle\!\rangle f J,$$

where

$$f = \mathbb{f}\cdot\mathbb{m} \tag{6.24}$$

denotes the *normal configurational force*. Also, by $(6.3)_2$,

$$\langle\!\langle \mathbf{C}\mathbb{m} + (V - \mathbf{u}\cdot\mathbb{m})\mathbf{q} \rangle\!\rangle \cdot [\![\mathbf{u}]\!] = -\mathbb{m}\cdot\langle\!\langle \mathbf{C}\mathbb{m} + (V - \mathbf{u}\cdot\mathbb{m})\mathbf{q} \rangle\!\rangle [\![\upsilon]\!] J.$$

Thus,

$$\mathbb{f}\cdot(\mathbb{v} - \langle\!\langle \mathbf{u} \rangle\!\rangle) + \langle\!\langle \mathbf{C}\mathbb{m} + (V - \mathbf{u}\cdot\mathbb{m})\mathbf{q} \rangle\!\rangle \cdot [\![\mathbf{u}]\!] = FJ, \tag{6.25}$$

with

$$F = \langle\!\langle \upsilon \rangle\!\rangle f - [\![\upsilon]\!] \mathbb{m}\cdot\langle\!\langle \mathbf{C}\mathbb{m} + (V - \mathbf{u}\cdot\mathbb{m})\mathbf{q} \rangle\!\rangle. \tag{6.26}$$

Finally, using (6.23) and (6.25) in (6.21), we arrive at the intrinsic expression

$$w(\mathcal{A}) = \int\limits_{\partial\mathcal{A}} \varphi(V_{\partial\mathcal{A}} - \mathbb{u}\cdot\mathbb{m}_{\partial\mathcal{A}})\,\mathrm{d}s - \int\limits_{\mathcal{A}} \Big\{ \varphi(KV - \mathsf{div}_s \mathbb{u}) + \mathbb{C}_{\tan}\colon \mathbb{D} \Big\}\,\mathrm{d}a - \int\limits_{\mathcal{A}} \Big\{ \mathbb{g}\cdot\mathbb{w} + FJ - \langle\!\langle \upsilon \rangle\!\rangle \mathbb{k}\cdot\mathsf{grad}_s J \Big\}\,\mathrm{d}a \tag{6.27}$$

for the total power expended on $\mathcal{A}$.

6.8 Imbalance of free energy

Since we neglect superficial distributions of momentum, the first and second laws for the interface reduce to an imbalance of free energy. Writing ψ for the *superficial free energy* (*density*), measured per unit area of $\mathcal{S}$, so that

$$\int\limits_{\mathcal{A}} \psi\,\mathrm{d}a \tag{6.28}$$

represents the net free energy of $\mathcal{A}$, the imbalance of free energy requires that, for any migrating interfacial pillbox $\mathcal{A}$,

$$\frac{\mathrm{d}}{\mathrm{d}t} \int\limits_{\mathcal{A}} \psi\,\mathrm{d}a \le w(\mathcal{A}), \tag{6.29}$$

with $w(\mathcal{A})$ given by (6.13) or its intrinsic equivalent (6.27). Thus, by the superficial transport theorem (5.18),

$$\int\limits_{\mathcal{A}} \Big\{ \mathring{\psi} + (\psi - \varphi)(KV - \mathsf{div}_s \mathbb{u}) \Big\}\,\mathrm{d}a + \int\limits_{\partial\mathcal{A}} (\psi - \varphi)(V_{\partial\mathcal{A}} - \mathbb{u}\cdot\mathbb{m}_{\partial\mathcal{A}})\,\mathrm{d}s$$
$$\le - \int\limits_{\mathcal{A}} \Big\{ \mathbb{C}_{\tan}\colon \mathbb{D} + \mathbb{g}\cdot\mathbb{w} + FJ - \langle\!\langle \upsilon \rangle\!\rangle \mathbb{k}\cdot\mathsf{grad}_s J \Big\}\,\mathrm{d}a. \tag{6.30}$$

This inequality can hold for all migrating pillboxes $\mathcal{A}$ only if the coefficient of $V_{\partial\mathcal{A}} - \mathbb{u}\cdot\mathbb{m}_{\partial\mathcal{A}}$ in the integral over $\partial\mathcal{A}$ vanishes. Thus, (6.18) becomes the *superficial Eshelby relation*

$$\mathbb{C}_{\tan} = \psi\,\mathbb{P} - \mathbb{T}_{\tan} \tag{6.31}$$

and (6.19) becomes

$$\mathbb{C} = \psi\,\mathbb{P} - \mathbb{T} + \mathbb{m}\otimes\mathbb{k}. \tag{6.32}$$

Moreover, the inequality (6.30) simplifies to

$$\int_{\mathcal{A}} \Big\{ \mathring{\psi} + \mathbb{C}_{\rm tan}\colon\mathbb{D} + \mathbb{g}\cdot\mathbb{w} + FJ - \langle\!\langle v\rangle\!\rangle\,\mathbb{k}\cdot\mathsf{grad}_s J \Big\}\,{\rm d}a \le 0 \tag{6.33}$$

or, equivalently, to the superficial dissipation inequality

$$\mathring{\psi} + \mathbb{C}_{\rm tan}\colon\mathbb{D} + \mathbb{g}\cdot\mathbb{w} + FJ - \langle\!\langle v\rangle\!\rangle\,\mathbb{k}\cdot\mathsf{grad}_s J \le 0. \tag{6.34}$$

subsectionThe configurational momentum balance revisited

Adding the configurational momentum balance (6.12) for the interface, decomposes into a normal component

$$\mathbb{m}\cdot\mathsf{div}_s\mathbb{C} + \mathbb{m}\cdot[\![\mathbf{C}\mathbb{m} + (V - \mathbf{u}\cdot\mathbb{m})\mathbf{q}]\!] + f = 0 \tag{6.35}$$

and a tangential component

$$\mathbb{P}\mathsf{div}_s\mathbb{C} + \mathbb{P}[\![\mathbf{C}\mathbb{m} + (V - \mathbf{u}\cdot\mathbb{m})\mathbf{q}]\!] + \mathbb{P}\mathbb{f} = \mathbf{0}. \tag{6.36}$$

We refer to (6.35) as the *normal configurational momentum balance*. While this balance is central to the description of the interface, the (nonintrinsic) tangential balance (6.36) is inconsequential to the theory.

An alternative version of the balance (6.35), involving explicitly the field F introduced in (6.26), can be obtained as follows.

Using (6.26) in (6.35) and multiplying through by $\langle\!\langle v\rangle\!\rangle$, taking advantage of the identity (5.7), and the relations (3.9), (3.10), and (4.3), we obtain

$$\langle\!\langle v\rangle\!\rangle\,\mathbb{m}\cdot\mathsf{div}_s\mathbb{C} + [\![v(\Psi + p - \mathbb{m}\cdot\mathbf{T}_{\rm dis}\mathbb{m})]\!] - [\![\tfrac{1}{2}|\mathbf{u}|^2 - (V - \mathbf{u}\cdot\mathbb{m})\mathbf{u}\cdot\mathbb{m}]\!] + \tfrac{1}{2}\sigma v^-|\dot{\mathbf{n}}|^2 + \sigma(v^-)^2 J\dot{\mathbf{n}}\cdot\mathbb{m} + F = 0$$

Thus, since, by $(5.8)_1$ and (6.3), $[\![\frac{1}{2}|\mathbf{u}|^2 - (V - \mathbf{u}\cdot\mathbb{m})\mathbf{u}\cdot\mathbb{m}]\!] = -\frac{1}{2}[\![v^2]\!]J^2 = -\langle\!\langle v\rangle\!\rangle[\![v]\!]J^2$, it follows that the normal combined momentum balance is equivalent to

$$\langle\!\langle v\rangle\!\rangle\,\mathbb{m}\cdot\mathsf{div}_s\mathbb{C} + [\![v(\Psi + p - \mathbb{m}\cdot\mathbf{T}_{\rm dis}\mathbb{m})]\!] + \langle\!\langle v\rangle\!\rangle[\![v]\!]J^2 + \tfrac{1}{2}\sigma v^-|\dot{\mathbf{n}}|^2 + \sigma(v^-)^2 J\dot{\mathbf{n}}\cdot\mathbb{m} + F = 0. \tag{6.37}$$

7 Superficial constitutive equations

Following Friedel (1926) and Oseen (1933), we assume that the superficial free-energy ψ is given constitutively as a properly invariant function of $\mathbf{n}$ and $\mathbb{m}$, so that

$$\psi = \hat{\psi}(\xi), \tag{7.1}$$

where $\xi = \mathbf{n}\cdot\mathbb{m}$ (cf. (5.23)). Then, by (5.24),

$$\mathring{\psi} = \frac{{\rm d}\hat{\psi}}{{\rm d}\xi}\,\mathring{\xi} = \frac{{\rm d}\hat{\psi}}{{\rm d}\xi}\big\{(\mathbb{m} - \xi\mathbf{n})\cdot\mathbb{w} - \langle\!\langle v\rangle\!\rangle(\mathbf{n} - \xi\mathbb{m})\cdot\mathsf{grad}_s J\big\}$$

and the superficial dissipation inequality (6.34) reduces to a residual inequality

$$\mathbb{C}_{\rm tan}\colon\mathbb{D} + \left\{\mathbb{g} + \frac{{\rm d}\hat{\psi}}{{\rm d}\xi}(\mathbb{m} - \xi\mathbf{n})\right\}\cdot\mathbb{w} + FJ - \langle\!\langle v\rangle\!\rangle\left\{\mathbb{k} + \frac{{\rm d}\hat{\psi}}{{\rm d}\xi}(\mathbf{n} - \xi\mathbb{m})\right\}\cdot\mathsf{grad}_s J \le 0. \tag{7.2}$$

The inequality (7.2) suggests the consideration of constitutive equations giving the symmetric part $\mathrm{Sym}(\mathbb{C}_{\rm tan})$ of $\mathbb{C}_{\rm tan}$, $\mathbb{g} + ({\rm d}\hat{\psi}/{\rm d}\xi)(\mathbb{m} - \xi\mathbf{n})$, F, and $\mathbb{k} + ({\rm d}\hat{\psi}/{\rm d}\xi)(\mathbf{n} - \xi\mathbb{m})$ as properly invariant functions of $\mathbf{n}$, $\mathbb{m}$, and the rates $\mathbb{D}$, $\mathbb{w}$, J, and $\mathsf{grad}_s J$. If we emulate the treatment of the bulk nematic phase and insist that those functions be linear in the rates $\mathbb{D}$, $\mathbb{w}$, J, and $\mathsf{grad}_s J$, we arrive at a description involving

29 independent constitutive moduli. For simplicity, we therefore restrict our attention to constitutive equations that result on neglecting coupling between the operative dissipative mechanisms or, equivalently, on replacing the inequality (7.2) with the more stringent requirements

$$\left.\begin{aligned} \mathbb{C}_{\tan}\!:\!\mathbb{D} &\leq 0,\\ \left\{\mathrm{g}+\frac{\mathrm{d}\psi}{\mathrm{d}\xi}(\mathbb{m}-\xi\mathbf{n})\right\}\cdot\mathbb{w} &\leq 0,\\ FJ &\leq 0,\\ \left\{\Bbbk+\frac{\mathrm{d}\psi}{\mathrm{d}\xi}(\mathbf{n}-\xi\mathbb{m})\right\}\cdot\mathsf{grad}_s J &\geq 0, \end{aligned}\right\} \tag{7.3}$$

and assuming that $\mathrm{Sym}(\mathbb{C}_{\tan})$ depends linearly on $\mathbb{D}$, $\mathrm{g}+(\mathrm{d}\psi/\mathrm{d}\xi)(\mathbb{m}-\xi\mathbf{n})$ depends linearly on $\mathbb{w}$, F depends linearly on J, and $\Bbbk+(\mathrm{d}\psi/\mathrm{d}\xi)(\mathbf{n}-\xi\mathbb{m})$ depends linearly on $\mathsf{grad}_s J$. Bearing in mind the relation (6.8) determining $\mathrm{g}\cdot\mathbf{n}$, these constitutive equations have the form[8]

$$\left.\begin{aligned} \mathrm{Sym}(\mathbb{C}_{\tan}) &= -(\lambda_1\mathsf{tr}\,\mathbb{D}+\lambda_2\mathbf{n}\cdot\mathbb{D}\mathbf{n})\mathbb{P}-(\lambda_3\mathsf{tr}\,\mathbb{D}+\lambda_4\mathbf{n}\cdot\mathbb{D}\mathbf{n})\mathbb{P}\mathbf{n}\otimes\mathbb{P}\mathbf{n}\\ &\quad -2\lambda_5\mathbb{D}-\tfrac{1}{2}\lambda_6(\mathbb{P}\mathbf{n}\otimes\mathbb{D}\mathbf{n}+\mathbb{D}\mathbf{n}\otimes\mathbb{P}\mathbf{n}),\\ \mathrm{g} &= (\boldsymbol{\alpha}\cdot\mathbf{n})\mathbf{n}-\frac{\mathrm{d}\psi}{\mathrm{d}\xi}(\mathbb{m}-\xi\mathbf{n})-\lambda_7\mathbb{w}-\lambda_8(\mathbb{w}\cdot\mathbb{m})(\mathbb{m}-\xi\mathbf{n}),\\ F &= -\lambda_9 J,\\ \Bbbk &= -\frac{\mathrm{d}\psi}{\mathrm{d}\xi}(\mathbf{n}-\xi\mathbb{m})+\lambda_{10}\mathsf{grad}_s J+\lambda_{11}(\mathbf{n}\cdot\mathsf{grad}_s J)\mathbb{P}\mathbf{n}, \end{aligned}\right\} \tag{7.4}$$

where the moduli $\lambda_1,\lambda_2,\ldots,\lambda_{11}$ may depend on ξ and — to ensure satisfaction of the inequalities (7.3) — must obey

$$\left.\begin{gathered} 4(\lambda_1+\lambda_5)+2(\lambda_2+\lambda_3+\tfrac{1}{2}\lambda_6)(1-\xi^2)+\lambda_4(1-\xi^2)^2\geq 0,\\ 4(\lambda_1+\lambda_5-\tfrac{1}{2}\lambda_6(1-\xi^2))\lambda_4\geq(\lambda_2+\lambda_3+\lambda_6)^2,\quad 4\lambda_5+\lambda_6(1-\xi^2)\geq 0,\\ \lambda_7\geq 0,\quad \lambda_7+\lambda_8\geq 0,\quad \lambda_9\geq 0,\quad \lambda_{10}\geq 0,\quad \lambda_{10}+\lambda_{11}\geq 0. \end{gathered}\right\} \tag{7.5}$$

Granted (7.4), the theory provides a supplemental constitutive equation for the interfacial Cauchy stress $\mathbb{T}$. To derive that relation, we first notice that, as a direct consequence of the expressions (6.11) determining the normal component $\mathbb{T}^{\top}\mathbb{m}$ and skew part $\frac{1}{2}(\mathbb{T}-\mathbb{T}^{\top})$ of $\mathbb{T}$ and the superficial Eshelby relation (6.32),

$$\mathbb{T}=\psi\mathbb{P}-\mathrm{Sym}(\mathbb{C}_{\tan})+\tfrac{1}{2}\mathbb{P}(\mathrm{g}\otimes\mathbf{n}-\mathbf{n}\otimes\mathrm{g})\mathbb{P}+\mathbb{m}\otimes((\mathrm{g}\cdot\mathbb{m})\mathbf{n}-\xi\mathrm{g}). \tag{7.6}$$

Thus, by $(7.4)_{1,2,4}$, we find by a direct calculation that

$$\mathbb{T}=\psi\mathbb{P}-\frac{\mathrm{d}\psi}{\mathrm{d}\xi}\mathbb{m}\otimes\mathbb{P}\mathbf{n}+\mathbb{T}_{\mathrm{dis}}, \tag{7.7}$$

with

$$\mathbb{T}_{\mathrm{dis}}=-\mathrm{Sym}(\mathbb{C}_{\tan}+\lambda_7\mathbb{m}\otimes(\xi\mathbb{w}-(\mathbb{w}\cdot\mathbb{m})\mathbf{n}))-\tfrac{1}{2}\lambda_7(\mathbb{w}\otimes\mathbf{n}-\mathbf{n}\otimes\mathbb{w})-\lambda_8(\mathbb{w}\cdot\mathbb{m})\mathbb{m}\otimes\mathbb{P}\mathbf{n}. \tag{7.8}$$

Thus, even for uncoupled constitutive equations of the form (7.4), the interfacial Cauchy stress includes terms involving not only the interfacial rate of stretch but also terms involving the invariant measure $\mathbb{w}$ of the rate at which $\mathbf{n}$ changes following the interface. Note that, by (7.7) and (7.8), the surface tension $\gamma=\frac{1}{2}\mathsf{tr}\,\mathbb{T}$ has the form

$$\gamma=\psi+\alpha_1\mathsf{tr}\,\mathbb{D}+\alpha_2\mathbf{n}\cdot\mathbb{D}_0\mathbf{n}, \tag{7.9}$$

[8]The constitutive equations should be compared with those provided by Rey [22, 23] and Poniewierski [20] or a *material* interface.

with

$$\left.\begin{aligned}\alpha_1 &= \lambda_1 + \lambda_5 + \tfrac{1}{2}\lambda_3(1-\xi^2),\\ \alpha_2 &= \lambda_2 + \tfrac{1}{2}\lambda_6 + \tfrac{1}{2}\lambda_4(1-\xi^2).\end{aligned}\right\} \tag{7.10}$$

Further, in view of the representation (6.32) of the interfacial configurational stress and the expression (7.7) for $\mathbb{T}$, it follows that

$$\mathbb{C} = \lambda_{10}\mathbb{m}\otimes\mathsf{grad}_s J + \lambda_{11}(\mathbf{n}\cdot\mathsf{grad}_s J)\mathbb{m}\otimes\mathbb{P}\mathbf{n} - \mathbb{T}_{\rm dis} \tag{7.11}$$

and, thus, that the interfacial configurational stress is of an entirely dissipative nature.

Direct calculations show that, granted (7.4), (7.7), and (7.11) the angular momentum balance (6.10) and the tangential component (6.36) are satisfied trivally.

8 Specialized interfacial evolution equations

Aside from the no-slip condition $(5.8)_1$ and the definition (6.2) of the interfacial mass flow, the general interfacial evolution equations of the theory are determined by inserting the constitutive equations (7.4) in the equations (6.4), (6.9), and (6.37) enforcing the balances of linear momentum, director momentum, and normal combined momentum. Instead of those equations, we present an illustrative specialization. In particular, we neglect all sources of dissipation excepting that associated with the exchange of mass between the phases. Thus, we assume that

$$\lambda_7 = \lambda_8 = \lambda_{10} = \lambda_{11} = 0 \tag{8.1}$$

and that

$$\lambda_9 = \lambda > 0. \tag{8.2}$$

The governing interfacial equations of the theory are then:

(i) the no-slip condition

$$\mathbb{P}[\![\mathbf{u}]\!] = \mathbf{0}; \tag{8.3}$$

(ii) the definition

$$J = \langle\!\langle \varrho(V - \mathbf{u}\cdot\mathbb{m})\rangle\!\rangle \tag{8.4}$$

of the interfacial mass flow;

(iii) the tangential component

$$\mathbb{P}(\mathsf{div}_s\mathbb{T}_{\rm dis} + [\![\mathbf{T}_{\rm dis}]\!]\mathbb{m}) = \mathbf{0} \tag{8.5}$$

of the linear momentum balance;

(iv) the normal component

$$\left\{\psi - \xi\frac{\mathrm{d}\psi}{\mathrm{d}\xi}\right\}K + \frac{\mathrm{d}^2\psi}{\mathrm{d}\xi^2}(\mathbb{K}\mathbf{n} - \mathbb{P}\mathbf{G}^{\top}\mathbb{m})\cdot\mathbf{n} - \frac{\mathrm{d}\psi}{\mathrm{d}\xi}\mathsf{tr}\,\mathbf{G} + \mathbb{m}\cdot\mathsf{div}_s\mathbb{T}_{\rm dis} = [\![p - \mathbb{m}\cdot\mathbf{T}_{\rm dis}\mathbb{m}]\!] + \sigma v^{-}J\mathbf{G}\mathbb{m}\cdot\dot{\mathbf{n}} + [\![v]\!]J^2 \tag{8.6}$$

of the linear momentum balance;

(v) the director momentum balance

$$\frac{\partial\Psi}{\partial\mathbf{G}}\mathbb{m} + \sigma(V - \mathbf{u}^{-}\cdot\mathbb{m})\dot{\mathbf{n}} = -\frac{\mathrm{d}\psi}{\mathrm{d}\xi}(\mathbb{m} - \xi\mathbf{n}); \tag{8.7}$$

(vi) and the normal configurational balance

$$\langle\!\langle v\rangle\!\rangle\mathbb{m}\cdot\mathsf{div}_s\mathbb{C} + [\![v(\Psi + p - \mathbb{m}\cdot\mathbf{T}_{\rm dis}\mathbb{m})]\!] + \langle\!\langle v\rangle\!\rangle[\![v]\!]J^2 + \tfrac{1}{2}\sigma v^{-}|\dot{\mathbf{n}}|^2 + \sigma(v^{-})^2 J\dot{\mathbf{n}}\cdot\mathbb{m} = \lambda J. \tag{8.8}$$

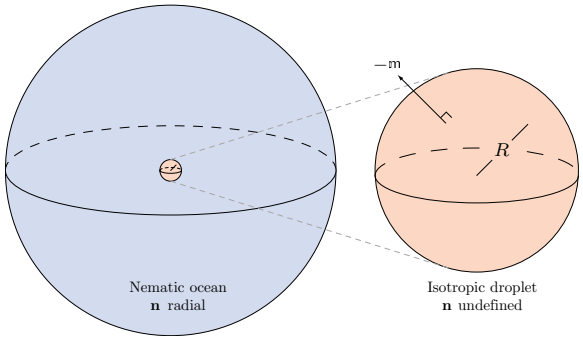

Figure 2: Schematic of an isotropic drop of radius R in an nematic ocean with radial director field. The interfacial unit normal $\mathtt{m}$ is directed outward from the nematic phase toward the origin.

In (8.5), (8.6), and (8.8), the limits $\mathbf{T}^{-}_{\rm dis}$ and $\mathbf{T}^{+}_{\rm dis}$ are determined from $(2.5)_1$ and $(4.1)_2$, respectively. Further, Ψ and $\partial\Psi/\partial\mathbf{G}$ are determined from (2.4). Also, since Ψ measures the free-energy density of the nematic phase relative to that of the isotropic phase, it follows that, in (8.8), $[\![v\Psi]\!] = -v^{-}\Psi$. Moreover, in (8.5) and (8.6), $\mathbb{T}_{\rm dis}$ is as given in (7.8).

When the densities of the two phases coincide, so that $[\![v]\!] = 0$, (8.3) and (8.4) are replaced by $[\![\mathbf{u}]\!] = \mathbf{0}$ and $J = \varrho(V - \mathbf{u}\cdot\mathtt{m})$, the tangential component of the linear momentum balance is unchanged from (8.5), and the normal component (8.6) of the linear momentum balance, the director momentum balance (8.7), and the combined normal momentum balance (8.8) admit obvious specializations.

9 Radial symmetry: Isotropic inclusion in a nematic ocean

In the absence of flow, Cermelli, Fried & Gurtin [5] considered the radially symmetric problem of an isotropic spherical drop growing (or receding) within a nematic ocean in which the director field is purely radial. Here, we reconsider that problem accounting for flow.

In the isotropic phase, the mesogens that make up a nematic liquid-crystalline fluid are randomly aligned. On the other hand, in the nematic phase, the mesogens display orientational order. Assuming that a closer packing of the mesogens accompanies such order, one expects the specific volume of the nematic phase to be slightly less than that of the isotropic phase. This expectation is confirmed by experiment and theory.[9] We therefore assume that

$$0 < \frac{[\![v]\!]}{v^{+}} \ll 1. \tag{9.1}$$

For simplicity, we neglect all external forces.

9.1 Kinematics

As in our previous work, we consider an isotropic spherical drop, with time-dependent radius R, surrounded by a nematic ocean with purely radial director field (Figure 2). Then

$$\mathbf{n}(\mathbf{x},t) = \frac{\mathbf{x}}{|\mathbf{x}|}, \qquad |\mathbf{x}| \geq R(t). \tag{9.2}$$

In addition, we assume that the velocity field has the particular form

$$\mathbf{u}(\mathbf{x},t) = \begin{cases} \mathbf{0}, & |\mathbf{x}| < R(t), \\ \dfrac{Q(t)\mathbf{x}}{|\mathbf{x}|^3}, & |\mathbf{x}| \geq R(t), \end{cases} \tag{9.3}$$

[9] For para-azoxyanisole (PAA), Maier & Saupe (1960) report that $[\![v]\!]/v^{+} \approx 0.0036$. For methoxybenzylidene butylaniline (MBBA), Press & Arrott [21] report that $[\![v]\!]/v^{+} \approx 0.0011$. For 4′-pentyl-4-biphenylcarbonitrile (5CB), Tintaru, Moldovan, Beica & Frunza [24] report that $\varrho^{-} \approx 1.0239$ g/cm^3 and $\varrho^{+} \approx 1.0214$ g/cm^3, whereby $[\![v]\!]/v^{+} \approx 0.0025$. Moreover, the molecular-statistical theory of Maier & Saupe [18] predicts values of $[\![v]\!]/v^{+}$ consistent with those obtained by experiment.

so that the isotropic drop is quiescent and a purely radial flow prevails in the nematic phase.

By (9.2), it follows that

$$\mathbf{G}(\mathbf{x},t)=\frac{1}{|\mathbf{x}|}\Big\{\mathbf{1}-\mathbf{n}(\mathbf{x},t)\otimes\mathbf{n}(\mathbf{x},t)\Big\},\qquad |\mathbf{x}|\geq R(t), \tag{9.4}$$

and

$$\dot{\mathbf{n}}(\mathbf{x},t)=\ddot{\mathbf{n}}(\mathbf{x},t)=\mathbf{0},\qquad |\mathbf{x}|\geq R(t). \tag{9.5}$$

Also, by (9.3),

$$\dot{\mathbf{u}}(\mathbf{x},t)=\begin{cases}\mathbf{0}, & |\mathbf{x}|<R(t),\\ \Big\{\dfrac{\dot{Q}(t)}{|\mathbf{x}|^2}-\dfrac{2Q^2(t)}{|\mathbf{x}|^5}\Big\}\dfrac{\mathbf{x}}{|\mathbf{x}|}, & |\mathbf{x}|\geq R(t),\end{cases} \tag{9.6}$$

and

$$\mathbf{L}(\mathbf{x},t)=\mathbf{D}(\mathbf{x},t)=\begin{cases}\mathbf{0}, & |\mathbf{x}|<R(t),\\ \dfrac{Q(t)}{|\mathbf{x}|^3}\Big\{\mathbf{1}-3\dfrac{\mathbf{x}}{|\mathbf{x}|}\otimes\dfrac{\mathbf{x}}{|\mathbf{x}|}\Big\}, & |\mathbf{x}|\geq R(t).\end{cases} \tag{9.7}$$

Moreover, consistent the convention that $\mathbb{m}$ is directed into the isotropic phase, we have

$$\mathbb{m}(\mathbf{x},t)=-\frac{\mathbf{x}}{R(t)},\quad \mathbb{K}(\mathbf{x},t)=\frac{1}{R(t)}\mathbb{P}(\mathbf{x},t),\quad K(\mathbf{x},t)=\frac{2}{R(t)},\quad V(\mathbf{x},t)=-\dot{R}(t),\quad \mathring{\mathbb{m}}(\mathbf{x},t)=\mathbf{0}, \tag{9.8}$$

on the isotropic-nematic interface $|\mathbf{x}|=R(t)$. Further,

$$\mathbf{n}(\mathbf{x},t)=-\mathbb{m}(\mathbf{x},t)=\frac{\mathbf{x}}{R(t)} \tag{9.9}$$

and, bearing in mind (9.4), (9.5), $(9.8)_5$, and (9.9),

$$\mathbf{G}(\mathbf{x},t)=\frac{1}{R(t)}\mathbb{P}(\mathbf{x},t)\qquad\text{and}\qquad \dot{\mathbf{n}}(\mathbf{x},t)=\mathring{\mathbf{n}}(\mathbf{x},t)=\mathbf{0} \tag{9.10}$$

on $|\mathbf{x}|=R(t)$. Also, by (5.8), (5.13), (9.2), (9.3), and $(9.10)_2$,

$$\left.\begin{aligned}\mathbf{u}^+(\mathbf{x},t)\cdot\mathbb{m}(\mathbf{x},t)=0,\qquad \mathbf{u}^-(\mathbf{x},t)\cdot\mathbb{m}(\mathbf{x},t)=-\frac{Q(t)}{R^2(t)},\\ \mathbb{u}(\mathbf{x},t)=\mathbf{0},\qquad \mathbb{v}(\mathbf{x},t)=\frac{\dot{R}(t)\mathbf{x}}{R(t)},\end{aligned}\right\} \tag{9.11}$$

where $\mathbb{v}$ is the materially intrinsic velocity-field, while, by (5.19), $(5.20)_1$, (5.23), (9.7), (9.9), and (9.10),

$$\mathbb{L}(\mathbf{x},t)=\mathbb{D}(\mathbf{x},t)=\frac{Q(t)}{|\mathbf{x}|^3}\mathbb{P}(\mathbf{x},t),\quad \mathbb{w}(\mathbf{x},t)=\mathbf{0},\quad\text{and}\quad \xi(\mathbf{x},t)=-1 \tag{9.12}$$

on $|\mathbf{x}|=R(t)$.

9.2 Bulk results

Granted that $\mathbf{u}$ is as defined in (9.3), the constraint $\mathsf{div}\,\mathbf{u}=0$ of incompressibility is satisified throughout both of the bulk phases.

Next, for the isotropic phase, it follows from (4.1) and (9.7) that $\mathbf{T}_{\rm dis}=\mathbf{0}$ for $|\mathbf{x}|<R(t)$. Thus, bearing in mind (9.6), the standard momentum balance $(4.2)_2$ implies that $\mathsf{grad}\,p=\mathbf{0}$ in the isotropic phase and, hence, that

$$p(\mathbf{x},t)=p^+(t),\qquad |\mathbf{x}|<R(t). \tag{9.13}$$

The pressure in the droplet is therefore uniform.

Next, for on the nematic phase, (9.2) and (9.4) imply that the free-energy density (2.4) specializes to

$$\Psi(\mathbf{x},t)=\hat{\Psi}(\mathbf{n}(\mathbf{x},t),\mathbf{G}(\mathbf{x},t))=\Psi_0+\frac{\kappa}{|\mathbf{x}|^2},\qquad |\mathbf{x}|\geq R(t),\tag{9.14}$$

where we have introduced

$$\kappa=2k_1-(k_2+k_4)\geq 0.\tag{9.15}$$

Further, direct calculations show that

$$\frac{\partial\hat{\Psi}(\mathbf{n}(\mathbf{x},t),\mathbf{G}(\mathbf{x},t))}{\partial\mathbf{G}}=\frac{\kappa}{|\mathbf{x}|}\Big\{\mathbf{1}-\mathbf{n}(\mathbf{x},t)\otimes\mathbf{n}(\mathbf{x},t)\Big\},\qquad |\mathbf{x}|\geq R(t),\tag{9.16}$$

and

$$\frac{\partial\hat{\Psi}(\mathbf{n}(\mathbf{x},t),\mathbf{G}(\mathbf{x},t))}{\partial\mathbf{n}}=\mathbf{0},\qquad |\mathbf{x}|\geq R(t).\tag{9.17}$$

As a consequence of (9.4), (9.14), and (9.16), we have the important identity

$$\mathsf{div}\Big\{\mathbf{G}^{\top}(\mathbf{x},t)\frac{\partial\hat{\Psi}(\mathbf{n}(\mathbf{x},t),\mathbf{G}(\mathbf{x},t))}{\partial\mathbf{G}}\Big\}=\mathsf{grad}\,\Psi(\mathbf{x},t),\qquad |\mathbf{x}|\geq R(t).\tag{9.18}$$

Further, using (9.5) and (9.7) in (2.5), we find that

$$\mathbf{T}_{\rm dis}=\frac{2(\mu_1+\mu_4)Q(t)}{|\mathbf{x}|^3}\Big\{\mathbf{1}-3\frac{\mathbf{x}}{|\mathbf{x}|}\otimes\frac{\mathbf{x}}{|\mathbf{x}|}\Big\},\qquad |\mathbf{x}|\geq R(t),\tag{9.19}$$

and

$$\mathbf{g}_{\rm dis}(\mathbf{x},t)=\mathbf{0},\qquad |\mathbf{x}|\geq R(t).\tag{9.20}$$

In view of (9.19), it follows that

$$\mathsf{div}\,\mathbf{T}_{\rm dis}(\mathbf{x},t)=\mathbf{0},\qquad |\mathbf{x}|\geq R(t).\tag{9.21}$$

By (9.6), (9.14), (9.18), and (9.21), the standard momentum balance $(2.3)_1$ implies that $\varrho^-\dot{\mathbf{u}}=-\mathsf{grad}\,(p+\Psi)$ in the nematic phase and, hence, bearing in mind (9.6), that

$$p(\mathbf{x},t)=p_\infty-\frac{\kappa}{|\mathbf{x}|^2}+\frac{\varrho^-}{|\mathbf{x}|}\Big\{\dot{Q}(t)-\frac{Q^2(t)}{2|\mathbf{x}|^3}\Big\},\qquad |\mathbf{x}|\geq R(t),\tag{9.22}$$

with p_∞ being the (constant) pressure in the far field. In contrast to the situation in the isotropic phase, the pressure in the nematic phase is therefore non-uniform.

Finally, using (9.4), (9.5), (9.16), and (9.17) in $(2.3)_2$, we find that the director momentum balance is satisfied identically on $|\mathbf{x}|>R(t)$ and, thus, throughout the nematic phase.

9.3 Interfacial mass balance

Using $(9.8)_1$ and $(9.11)_{1,2}$ in the interfacial mass balance (6.1), we obtain

$$Q=-\frac{[\![\varrho]\!]R^2\dot{R}}{\varrho^-}=\frac{[\![v]\!]R^2\dot{R}}{v^+},\tag{9.23}$$

which determines Q in terms of the droplet radius R. Using (9.23) in $(9.11)_2$ and recalling from (9.3) that $\mathbf{u}$ is radial, we obtain

$$\mathbf{u}^-=-\frac{[\![v]\!]\dot{R}}{v^+}\mathfrak{m}\tag{9.24}$$

and thus conclude that a liquid particle residing instantaneously on a phase interface that is moving outward must therefore move outward radially with scalar normal velocity $-[\![v]\!]\dot{R}/v^+$ (since $\mathfrak{m}$ is directed into the inclusion, the normal velocity is negative for an outward motion). Analogous to what occurs (Cermelli & Fried [4]) for a migrating disclination, a backflow therefore accompanies the motion of the phase interface. This suggests that an indirect measurement of the ratio $[\![v]\!]/v^+$ and, thus, of the density difference between the phases might be achieved as a by-product of a backflow measurement. Moreover, by $(6.3)_2$, the mass flow across the interface is given by

$$J=-\frac{\dot{R}}{v^+}.\tag{9.25}$$

9.4 Interfacial linear momentum balance

Using (9.23) in $(9.12)_1$ to give

$$\mathbb{D} = \frac{[\![v]\!]\dot{R}}{v^+R}\,\mathbb{P} \tag{9.26}$$

and bearing in mind (9.9) and $(9.12)_2$, we find from (7.7) and (7.8) that, for the purely radial problem under consideration, the interfacial Cauchy stress reduces to a pure tension of the form

$$\mathbb{T} = \left\{\sigma + \frac{2[\![v]\!](\lambda_1+\lambda_5)\dot{R}}{v^+R}\right\}\mathbb{P}, \tag{9.27}$$

with

$$\gamma_0 = \psi(-1). \tag{9.28}$$

Moreover, using (9.23) in the expressions (9.19) and (9.22) for the dissipative stress and pressure in the nematic phase, we find that their interfacial limits are given by

$$\mathbf{T}^-_{\rm dis} = \frac{2[\![v]\!](\mu_1+\mu_4)\dot{R}}{v^+R}\left\{\mathbf{1} - 3\mathbb{m}\otimes\mathbb{m}\right\} \tag{9.29}$$

and

$$p^- = p_\infty - \frac{\kappa}{R^2} + \frac{[\![v]\!]}{v^+v^-}\left\{R\ddot{R} + \left(2 - \frac{[\![v]\!]}{2v^+}\right)\dot{R}^2\right\}. \tag{9.30}$$

Further, since $[\![(V-\mathbf{u}\cdot\mathbb{m})\mathbf{p}]\!] = J[\![\mathbf{u}]\!]$, it follows from $(9.11)_{1,2}$, (9.24), and (9.25) that

$$[\![(V-\mathbf{u}\cdot\mathbb{m})\mathbf{p}]\!] = -\frac{[\![v]\!]\dot{R}^2}{v^+v^+} \tag{9.31}$$

Using (9.27), (9.29), (9.30), and (9.31) in the tangential and normal components (8.5) and (8.6) of the interfacial linear momentum balance, recalling $\mathbf{T}_{\rm dis} = \mathbf{0}$ in the isotropic phase, and noting, from (5.6) and $(9.8)_3$, that $\mathsf{div}_{\rm s}\mathbb{P} = K\mathbb{m} = 2\mathbb{m}/R$, we find that (8.5) is satisfied trivially and that (8.6) yields an expression

$$p^+ = p_\infty + \frac{2\gamma_0}{R} - \frac{\kappa}{R^2} + \frac{[\![v]\!]}{v^+v^-}\left\{R\ddot{R} + \left(2-\frac{[\![v]\!]}{2v^+}\right)\dot{R}^2\right\} + \frac{4[\![v]\!](\mu_1+\mu_4)\dot{R}}{v^+R} - \frac{[\![v]\!]\dot{R}^2}{v^+v^+} + \frac{4[\![v]\!](\lambda_1+\lambda_5)\dot{R}}{v^+R^2} \tag{9.32}$$

for the uniform pressure p^+ in the isotropic phase in terms of the droplet radius.

9.5 Interfacial director momentum balance

By (9.9) and $(9.12)_3$,

$$\frac{\mathrm{d}\psi}{\mathrm{d}\xi}(\mathbb{m} - \xi\mathbf{n}) = \mathbf{0}. \tag{9.33}$$

Further, evaluating (9.16) on the interface and using $(9.10)_1$, we find that

$$\frac{\partial\Psi}{\partial\mathbf{G}}\mathbb{m} = \mathbf{0} \tag{9.34}$$

on the interface. Also, by $(9.10)_2$,

$$\sigma(V-\mathbf{u}^-\cdot\mathbb{m})\dot{\mathbf{n}} = \mathbf{0} \tag{9.35}$$

on the interface. In view of (9.33), (9.34), and (9.35), the interfacial director momentum balance (8.7) is satisfied identically.

9.6 Normal configurational balance

Using (9.9), $(9.10)_2$, $(9.12)_{2,3}$, and (9.26) in $(7.4)_2$, we find that $\mathbb{P}\mathbf{g} = \mathbf{0}$ and that $\xi\mathbf{g} = (\mathbf{g}\cdot\mathbb{m})\mathbf{n}$ and, thus, from (6.32), (7.7), and (7.11), that

$$\mathbb{C} = \mathbb{C}_{\tan} = -\frac{2[\![v]\!](\lambda_1+\lambda_5)\dot{R}}{v^+R}\,\mathbb{P}. \tag{9.36}$$

Thus, by (5.6), (9.14), (9.24), (9.25), (9.29), and (9.30), the normal combined momentum balance (6.37) specializes to

$$p^+ = \frac{v^-}{v^+}\left\{\Psi_0 + p_\infty + \frac{[\![v]\!]}{v^+v^-}\left\{R\ddot{R} + \left(2 - \frac{[\![v]\!]}{2v^+}\right)\dot{R}^2\right\} + \frac{4[\![v]\!](\mu_1+\mu_4)\dot{R}}{v^+R}\right\}$$
$$+ \frac{\langle\!\langle v\rangle\!\rangle[\![v]\!]\dot{R}}{v^+v^+}\left\{\frac{4(\lambda_1+\lambda_5)}{R^2} - \frac{\dot{R}}{v^+}\right\} - \frac{\lambda_9\dot{R}}{v^+v^+}, \tag{9.37}$$

which, like (9.32), provides an expression for p^+ in terms of R.

9.7 Droplet evolution equation

Eliminating p^+ between (9.32) and (9.37), we arrive at a second-order nonlinear differential equation

$$\frac{[\![v]\!]^2}{v^+v^-}\left\{R\ddot{R} + \frac{3\dot{R}^2}{2} + \frac{4v^-(\mu_1+\mu_4)\dot{R}}{R} + \frac{2v^-(\lambda_1+\lambda_5)\dot{R}}{R^2}\right\} + \frac{\lambda_9\dot{R}}{v^+} = v^-\Psi_0 - [\![v]\!]p_\infty - v^+\left\{\frac{2\gamma_0}{R} - \frac{\kappa}{R^2}\right\}. \tag{9.38}$$

When $[\![v]\!] = 0$, this equation reduces to an equation with structure identical to that of the equation derived and studied by Cermelli, Fried & Gurtin [5] for the droplet evolution problem without flow.

Introducing the dimensionless variables

$$r = R/L \qquad \text{and} \qquad \tau = t/T,$$

with $L > 0$ a characteristic length and $T > 0$ a characteristic time, and letting

$$\epsilon = \frac{[\![v]\!]}{v^+}, \tag{9.39}$$

we may rewrite (9.38) in the simpler form

$$\beta_*\dot{r} = \Psi_* - \frac{2\gamma_*}{r} + \frac{\kappa_*}{r^2} - \epsilon(1+\Psi_*) - \epsilon^2\left\{\alpha_*\left(r\ddot{r} + \frac{3\dot{r}^2}{2}\right) + \frac{4\mu_*\dot{r}}{r} + \frac{2\lambda_*\dot{r}}{r^2}\right\}, \tag{9.40}$$

where the superposed dot now stands for differentiation with respect to τ and the parameters α_*, μ_*. λ_*, β_*, Ψ_*, γ_*, and κ_* are defined by

$$\left.\begin{aligned} \alpha_* = \frac{L^2}{v^-p_\infty T^2}, \quad \mu_* = \frac{\mu_1+\mu_4}{p_\infty T}, \quad \lambda_* = \frac{\lambda_1+\lambda_5}{p_\infty LT}, \\ \beta_* = \frac{\lambda_9 L}{v^+v^+p_\infty T}, \quad \Psi_* = \frac{v^-\Psi_0}{p_\infty v^+}, \quad \gamma_* = \frac{\gamma_0}{p_\infty L}, \quad \kappa_* = \frac{\kappa}{p_\infty L^2}. \end{aligned}\right\} \tag{9.41}$$

We now study equation (9.40) in two steps:

Case (a). Assume that the densities of the nematic and isotropic phases are almost coincident, so that

$$[\![v]\!] \ll v^+,$$

and neglect the term multiplying ϵ^2 in (9.40): the evolution equation for the interface then reduces to

$$\beta_*\dot{r} = \pi_* - \frac{2\gamma_*}{r} + \frac{\kappa_*}{r^2}, \tag{9.42}$$

with

$$\pi_* = \Psi_* - \epsilon(1+\Psi_*).$$

We have three regimes:

- When $\pi_* < 0$, i.e. when $p_\infty > \upsilon^- \Psi_0 / [\![\upsilon]\!]$, there is a stable radius for the isotropic inclusion, given by the expression
$$r_0 = \frac{\sqrt{\gamma_*^2 + \kappa_* |\pi_*|} - \gamma_*}{|\pi_*|}.$$
Note the competition between the externally applied pressure p_∞ and the free energy difference Ψ_0. When Ψ_0 is negative, the energy of the nematic phase is lower energy than that of isotropic phase and the drop should grow. On the other hand, the presence of an external pressure stabilizes finite-radius drops, and, since r_0 is a decreasing function of $|\pi_*|$, it follows that an increase of pressure tends to decrease the droplet radius. However, the droplet radius never vanishes because, in the limit as r_0 approaches zero, the droplet becomes a hedgehog defect and the associated defect energy must be taken into account. Moreover, note that for Ψ_0 positive high pressures stabilize a droplet of the isotropic phase surrounded by the nematic phase.

- When $0 < \pi_* < \gamma_*^2/\kappa_*$, i.e. when $(\upsilon^- \Psi_0 - \upsilon^+ \gamma_*^2)/[\![\upsilon]\!]\kappa_* < p_\infty < \upsilon^- \Psi_*/[\![\upsilon]\!]$, there are two equilibrium radii for the inclusion:
$$r_{0,1} = \frac{\gamma_* \pm \sqrt{\gamma_*^2 - \kappa_* \pi_*}}{\pi_*}.$$
The smallest of these radii is stable (since defect energy prohibits the disappearance of the droplet) but the largest is unstable. Hence, sufficiently large droplets grow without bound and the liquid becomes eventually isotropic.

- Finally, when $\gamma_*^2/\kappa_* < \pi_*$, i.e. when $p_\infty < (\upsilon^- \Psi_0 - \upsilon^+ \gamma_*^2)/[\![\upsilon]\!]\kappa_*$, there is no equilibrium radius and the isotropic droplet grows without bound.

Case (b). Consider now the full nonlinear ordinary differential equation (9.40). The equilibria of this equation are the same as those of (9.42).

Let $r_{\rm eq}$ be a generic equilibrium radius for the inclusion, as determined in case (a), and linearize (9.40) in a neighborhood of $r_{\rm eq}$, letting $Y = r - r_{\rm eq}$. We obtain a linear second order problem of the form
$$a_1 \ddot{Y} + a_2 \dot{Y} + a_3 Y = 0, \tag{9.43}$$
with
$$a_1 = \epsilon^2 \alpha_* r_{\rm eq}, \qquad a_2 = \epsilon^2 \left(\frac{4\mu_*}{r_{\rm eq}} + \frac{2\lambda_*}{r_{\rm eq}^2} + \beta_* \right), \qquad a_3 = -\frac{2\gamma_*}{r_{\rm eq}^2} + \frac{2\kappa_*}{r_{\rm eq}^3}.$$
The stability of the equilibrium solution may be discussed by studying the sign of the real part of the solution of the characteristic equation associated with (9.43). There are three possibilities:

- When $a_3 < 0$, i.e. when the equilibrium radius $r_{\rm eq}$ is unstable for the reduced equation (9.42), we have
$$\frac{-a_2 + \sqrt{a_2^2 + 4a_1|a_3|}}{2a_1} > 0,$$
so that $Y = 0$, i.e. $r = r_{\rm eq}$, is unstable also for the fully nonlinear equation (9.40).

- When $0 < a_3 < a_2^2/4a_1$, i.e. when the equilibrium radius $r_{\rm eq}$ is stable for the reduced equation (9.42), we have
$$\frac{-a_2 \pm \sqrt{a_2^2 + 4a_1|a_3|}}{2a_1} < 0,$$
so that $Y = 0$, i.e. when $r = r_{\rm eq}$, is stable also for the fully nonlinear equation (9.40).

- When $a_2^2/4a_1 < a_3$, again $r_{\rm eq}$ is stable for the reduced equation (9.42) and we have
$$\frac{-a_2 \pm i\sqrt{4a_1 a_3 - a_2^2}}{2a_1},$$
which is complex with negative real part. Thus, again, $r = r_{\rm eq}$ is stable for the fully nonlinear equation (9.40), but now the solution develops exponentially decaying oscillations near equilibrium.

For the droplet problem in the absence of flow, Cermelli, Fried & Gurtin [5] observed the existence of different time scales characterizing the evolution of the droplet. In particular, focusing on the case where the isotropic-to-nematic transition is favored, it was found that immediately subsequent to nucleation the droplet grows with the cube root of time. This is followed by a regime in which the droplet grows like the square root of time. Finally, for sufficiently late stages of growth, the droplet grow linearly with time. Due to the presence of the effects associated with inertia, the viscosities of the nematic phase, and the dilatational viscosity of the interface, we expect the more general evolution equation to display even more time scales. We leave the study of these effects for a future work.

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